

Electronic Supporting Information to:

**μ_3 -Oxo stabilized by three metal cations is a sufficient nucleophile
for enzymatic hydrolysis of phosphate monoesters**

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1. Supplementary table, figures, and schemes

Table S1. Energies of enzyme-methyl phosphate complexes in various electronic states

entry	multiplicity	spin			energy (kcal/mol)
		Fe _A	Fe _B	O _μ	
1	1	3.94	-4.09	-0.21	0.0
2	1	1.09	-0.93	-0.11	50.2
3	1	3.56	-2.76	-0.08	35.5
4	3	1.08	0.92	0.11	50.1
5	6	3.54	2.87	0.12	38.7
6	11	3.96	4.10	0.62	5.4

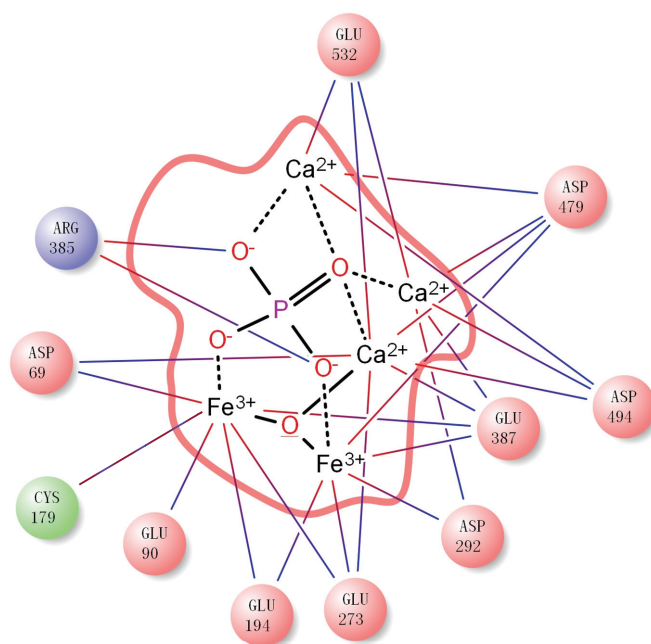


Fig. S1 Schematic ligand interactions in the PhoX active site. Coordinates from PDB entry 4ALF were used to generate the picture.

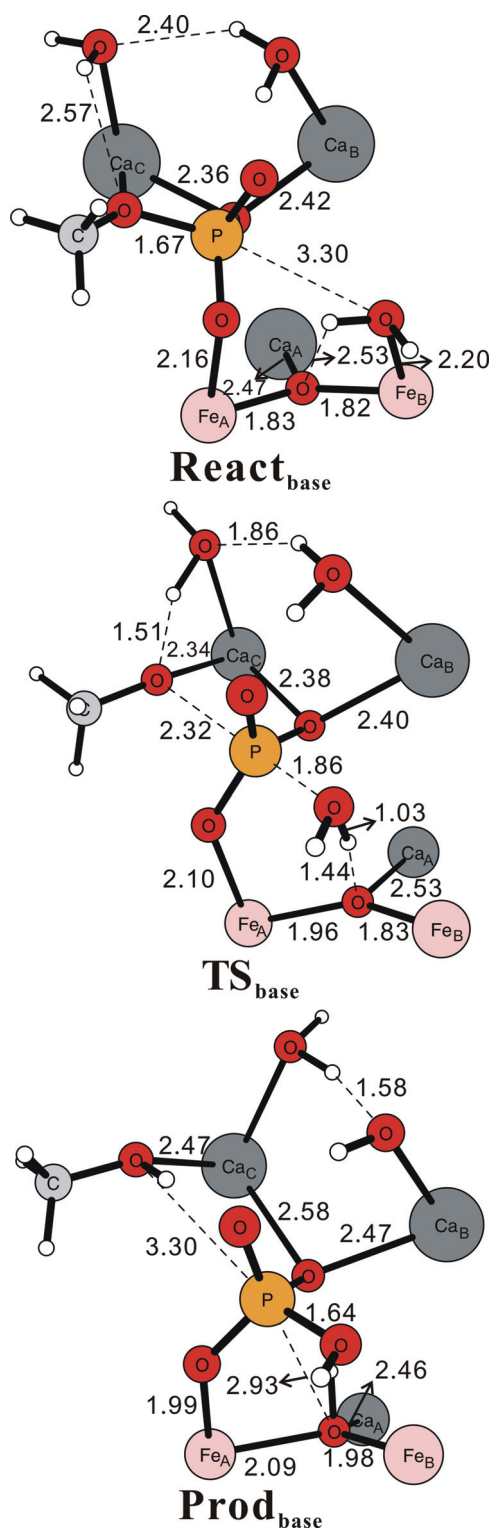
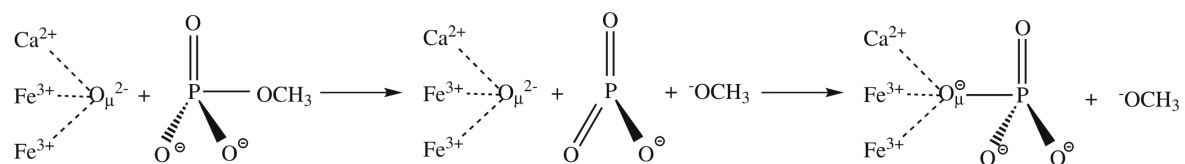
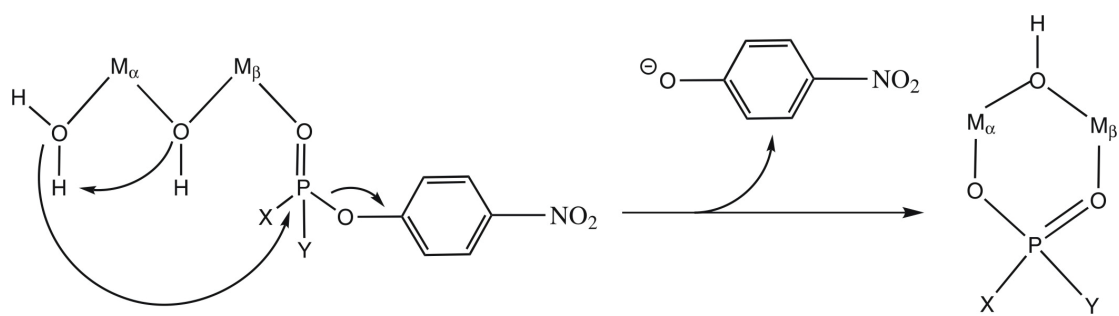


Fig. S2 Optimized structures of reactant (**React_{base}**), transition state (**TS_{base}**), and product (**Prod_{base}**) for the base mechanism in the PhoX-catalyzed hydrolysis of methyl phosphate. For clarity, ligands are omitted except for some key water molecules. All distances are indicated in angstrom (Å).



Scheme S1 Schematic dissociative mechanism for the PhoX-catalyzed hydrolysis of methyl phosphate.



Scheme S2 Schematic base mechanism for the phosphotriesterase (PTE) reaction.

2. Cartesian coordinates and absolute anergies of all optimized structures

The abbreviations used here are consistent with those in the text. All energies here are the absolute energies in hartree. Frequencies are given in cm^{-1} .

React_{me}

Energy with the medium-sized basis set:	-5503.08197
Solution energy with the medium-sized basis set:	-5503.16761
Energy with larger basis sets:	-5505.13992
Zero-point energy:	1.60918
Dispersion effect:	-0.33547

C	-6.8650001809	-6.1059998998	20.3889998995
C	-7.6524593855	-5.0462579846	19.6160598945
C	-9.1498222945	-5.3822348850	19.4807977049
O	-9.4695550933	-6.5955635430	19.4837593991
O	-9.9119395559	-4.3725851016	19.3510332778
H	-7.2112841389	-6.1723185558	21.4282975791
H	-7.5606023941	-4.0582834917	20.0822761412
H	-7.2483558715	-4.9456660690	18.5966704821
C	-7.4140000731	-0.0290000313	21.7369999778
C	-8.7746126422	-0.7195704367	21.9565587206
C	-9.5598117231	-0.8647600640	20.6457446081
C	-10.9649682624	-1.4670809317	20.7360613312
O	-11.3503996144	-2.0219412053	21.7988868615
O	-11.6556935186	-1.3410072242	19.6746099392
H	-6.7981171631	-0.5956386236	21.0271583232
H	-8.6147643413	-1.7136554413	22.3945773102
H	-9.3704492947	-0.1492063656	22.6828708583
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C	-8.8830000597	-1.7600000000	16.9099999801
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H	-15.6795538725	0.3453089694	20.8389453121
H	-16.9870859011	0.5287742342	19.6373909498

TS_{me}

Energy with the medium-sized basis set:	-5503.06794
Solution energy with the medium-sized basis set:	-5503.15184
Energy with larger basis sets:	-5505.12488
Zero-point energy:	1.60723
Imaginary frequency:	-116.8327
Dispersion effect:	-0.33149

C	-6.8650000000	-6.1060000000	20.3890000000
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C	-17.6149000000	-4.9224530000	15.7559600000
O	-18.5884870000	-5.5322110000	16.2611920000
O	-16.7145380000	-4.3843190000	16.5166110000
H	-15.7211750000	-4.8725950000	12.0602290000
H	-17.1686410000	-6.9625440000	13.8125340000
H	-15.6917390000	-6.1219340000	14.2657920000
H	-16.9622400000	-3.9109930000	13.9892170000
H	-18.4533780000	-4.8643230000	13.7942450000
C	-16.3930000000	-9.8490000000	16.0550000000
C	-16.8793000000	-8.8450620000	17.0990220000
C	-15.9069580000	-7.6988390000	17.3706750000
O	-14.7871840000	-7.6609210000	16.8159320000
O	-16.3061760000	-6.7887780000	18.1841750000

H	-16.2251740000	-9.3568640000	15.0915510000
H	-17.8300710000	-8.3895800000	16.7863390000
H	-17.0759510000	-9.3408170000	18.0609620000
C	-17.5420000000	-9.6660000000	21.8140000000
C	-17.3935960000	-8.2074750000	22.2862430000
C	-18.0875970000	-7.1767140000	21.4051520000
O	-19.3304230000	-7.2914120000	21.1787500000
O	-17.3863450000	-6.2095900000	20.9562540000
H	-18.5976870000	-9.9499860000	21.7444170000
H	-17.8169700000	-8.1099400000	23.2966160000
H	-16.3382450000	-7.9435790000	22.3336550000
C	-14.0160000000	-9.9710000000	25.1560000000
C	-14.6348420000	-8.8707780000	24.3073340000
C	-14.1536560000	-7.4610360000	24.6997020000
C	-14.6554080000	-6.4402820000	23.6979230000
O	-15.3864170000	-5.4773260000	24.0749130000
O	-14.3554500000	-6.6342210000	22.4700260000
H	-14.3793710000	-10.9626610000	24.8576850000
H	-14.3908870000	-9.0333240000	23.2518110000
H	-15.7279030000	-8.9165570000	24.3937930000
H	-14.4927530000	-7.1924730000	25.7058970000
H	-13.0573590000	-7.4262180000	24.6823210000
C	-10.0720000000	-10.4520000000	20.3670000000
C	-11.1684030000	-9.4170880000	20.6846140000
O	-11.3389890000	-8.4898990000	19.5822540000
C	-10.9042280000	-8.6639880000	21.9946810000
H	-10.2875550000	-10.9507810000	19.4163770000
H	-12.1309570000	-9.9427390000	20.7553600000
H	-10.6534420000	-7.7720730000	19.6398220000
H	-11.7192860000	-7.9669230000	22.2154670000
H	-10.8061790000	-9.3646330000	22.8342190000
H	-9.9802860000	-8.0815600000	21.9101450000
C	-9.3520000000	-7.6870000000	26.4130000000
C	-9.8006690000	-6.9118690000	25.1614720000
C	-10.0413430000	-5.4107360000	25.4271240000
C	-10.7090540000	-4.7016110000	24.2461200000
O	-11.7116420000	-5.1922470000	23.7108240000
N	-10.1693030000	-3.5277250000	23.8620470000
H	-8.4122320000	-7.2890870000	26.8182170000
H	-9.0514170000	-7.0223560000	24.3662200000
H	-10.7279530000	-7.3414100000	24.7689220000
H	-10.7212100000	-5.3043450000	26.2854770000
H	-9.0992790000	-4.9169340000	25.7025470000
H	-9.3404210000	-3.1780220000	24.3134910000

H	-10.5628090000	-2.9838370000	23.0837930000
P	-15.7528820000	-2.4641980000	19.1977890000
O	-16.1026600000	-3.9470700000	19.5881650000
O	-14.5353260000	-1.8552490000	19.9115520000
O	-16.5671050000	-1.8065560000	18.0383150000
O	-17.0183230000	-1.7971010000	20.4111660000
Ca	-14.1777590000	-5.4590540000	17.8889230000
Ca	-17.9375780000	-5.1812820000	18.6617450000
Ca	-15.6209900000	-4.7191780000	21.7731640000
Fe	-12.9737830000	-2.0961840000	18.4439250000
Fe	-15.6806770000	-2.4783150000	16.3353470000
O	-14.5565310000	-3.0678030000	17.7611170000
O	-12.4417360000	-4.1374230000	19.1972410000
O	-13.3292890000	-3.8904730000	21.8769060000
O	-17.5549910000	-3.2999100000	22.2749550000
O	-19.5685750000	-4.4481350000	20.6790240000
O	-19.9478720000	-6.6222420000	18.7060560000
O	-13.5446920000	-6.9418470000	19.7627820000
H	-6.9051890000	-6.9400370000	19.6814220000
H	-5.8185450000	-5.7933290000	20.5036670000
H	-7.5801010000	1.0261900000	21.4843230000
H	-6.7995740000	-0.0635630000	22.6454060000
H	-8.6127640000	-2.3124180000	16.0020730000
H	-8.1122560000	-0.9958050000	17.0875000000
H	-12.1378250000	3.6991290000	15.6616840000
H	-10.9051690000	2.8607100000	14.7024820000
H	-11.1613020000	-2.7332890000	12.1083770000
H	-12.3329050000	-1.5838340000	11.4299260000
H	-19.1414410000	-0.3282140000	12.4880910000
H	-17.5709970000	0.1121690000	11.7780150000
H	-21.3440490000	-4.0157040000	11.5992700000
H	-22.9927080000	-3.4812480000	11.9765330000
H	-15.6759310000	-6.6270580000	11.8025910000
H	-17.1957660000	-5.7372560000	11.5950990000
H	-15.4406760000	-10.2939910000	16.3591500000
H	-17.1245330000	-10.6539360000	15.9101360000
H	-17.0831430000	-9.8054670000	20.8279690000
H	-17.0440160000	-10.3451100000	22.5145640000
H	-12.9222390000	-9.9761040000	25.0593750000
H	-14.2508230000	-9.8391760000	26.2210780000
H	-9.0978410000	-9.9553200000	20.2819570000
H	-10.0099970000	-11.2095160000	21.1585450000
H	-10.1089900000	-7.6275350000	27.2056640000
H	-9.1928450000	-8.7459450000	26.1793460000

H	-19.8457120000	-7.0745630000	19.5846060000
H	-19.9156570000	-7.2862640000	18.0072440000
H	-18.9651220000	-4.0415210000	21.3434000000
H	-19.6611670000	-5.3856540000	20.9619310000
H	-17.3445050000	-2.5639350000	21.5364680000
H	-17.7276290000	-2.8691830000	23.1198540000
H	-12.8725000000	-3.0196560000	21.7774420000
H	-12.7410270000	-4.4123310000	22.4765980000
H	-11.3934120000	-4.3044430000	19.2053850000
H	-12.6946530000	-4.1832830000	20.1451340000
H	-12.7460890000	-7.5263520000	19.6683460000
H	-13.7663830000	-6.9758160000	20.7093880000
C	-16.9600060000	-0.3893190000	20.6322640000
H	-17.7428080000	-0.1139970000	21.3516850000
H	-15.9795900000	-0.0954080000	21.0221040000
H	-17.1407020000	0.1429660000	19.6924510000

Int_{me}

Energy with the medium-sized basis set:	-5503.09839
Solution energy with the medium-sized basis set:	-5503.18264
Energy with larger basis sets:	-5505.15824
Zero-point energy:	1.60725
Dispersion effect:	-0.32895

C	-6.8650001871	-6.1059998964	20.3889999013
C	-7.7345378217	-4.9777027944	19.8267261811
C	-9.2149787382	-5.3587178723	19.6202330768
O	-9.5276872641	-6.5665299223	19.6945589609
O	-9.9775772457	-4.3647981127	19.3669157135
H	-7.2092407454	-6.4048425114	21.3859012862
H	-7.7022020336	-4.0939266035	20.4779220488
H	-7.3471838778	-4.6449745418	18.8517136578
C	-7.4140001322	-0.0290000549	21.7369999513
C	-8.8067492222	-0.6335716655	21.9858775141
C	-9.4864724505	-1.0007697127	20.6610160213
C	-10.9362290220	-1.4645391394	20.7353793723
O	-11.4025471030	-2.0015809500	21.7584346272
O	-11.5912649462	-1.2465654910	19.6445269618
H	-6.7722683156	-0.7339878719	21.1930088517
H	-8.7194088333	-1.5270714012	22.6175228371
H	-9.4316162526	0.0810767252	22.5390682876
H	-9.4471381211	-0.1490130459	19.9710865941
H	-8.9411500636	-1.8213812998	20.1719082979

C	-8.8830000929	-1.7600000158	16.9099999935
C	-10.2549271867	-1.1257342674	16.6994257336
S	-11.5481626260	-2.4266981596	16.5065528978
H	-8.9004142626	-2.4344967940	17.7717326645
H	-10.5220340628	-0.4909255490	17.5468032446
H	-10.2644314979	-0.5178078487	15.7885386675
C	-11.9689999961	2.8629998487	14.9700001475
C	-12.3810573166	1.5172870992	15.5809099982
C	-13.8532859067	1.4631262189	16.0561374952
C	-14.1650280717	0.0831700006	16.6323512194
O	-13.5549495227	-0.2543667001	17.6747614159
O	-14.9939059523	-0.6340892799	15.9682172892
H	-12.5758635536	3.1053589651	14.0877468170
H	-12.2187846778	0.7173469919	14.8451691703
H	-11.7407292048	1.2904075127	16.4391921477
H	-14.0114725352	2.2133729047	16.8423043725
H	-14.5369003089	1.6785822739	15.2283037660
C	-12.1639999324	-2.3060000211	12.2389999989
C	-13.2655846211	-3.3799161350	12.2407442696
C	-13.1280216436	-4.4015028381	13.3872413166
C	-13.8598420560	-4.1263185721	14.7077590305
O	-14.7125420240	-3.1544887172	14.7350315742
O	-13.6099322834	-4.9002433917	15.6520175394
H	-12.1708633469	-1.7453878191	13.1810865953
H	-14.2476465990	-2.8967825786	12.3072976098
H	-13.2391452355	-3.9165378492	11.2813083385
H	-13.4892895946	-5.3877955166	13.0647826947
H	-12.0733433716	-4.5507025524	13.6515159162
C	-18.0649999077	-0.5230001738	12.5230003126
C	-17.6051741784	-0.0925990723	13.9296791987
C	-18.3062341511	-0.9726785832	14.9504591409
O	-19.5315018530	-0.8230809463	15.1279265338
O	-17.6311453919	-1.9093262512	15.5308926600
H	-17.7752886035	-1.5602728928	12.3165808233
H	-16.5214860597	-0.1738879201	14.0382938908
H	-17.8966086520	0.9495169905	14.1091367770
C	-21.9319999490	-3.3250000019	12.2140001743
C	-21.6613908822	-3.5711213221	13.7122610523
C	-22.4976926534	-2.6535089742	14.6273209321
C	-22.3465134134	-2.9380310822	16.1344466356
N	-20.9999861106	-2.6005008040	16.6100708510
C	-20.5607379844	-2.8465814574	17.8419971896
N	-21.3530681574	-3.3277998713	18.8109241632
N	-19.2516204636	-2.6435727894	18.1513972770

H	-21.6915205351	-2.2908489751	11.9368125795
H	-21.8771214168	-4.6212497160	13.9577732254
H	-20.5958870020	-3.4175903479	13.9216365883
H	-22.2334400843	-1.6046291744	14.4353771610
H	-23.5627761913	-2.7633716662	14.3767042218
H	-23.0996396539	-2.3540598833	16.6872196688
H	-22.5423118811	-4.0027958544	16.3290311738
H	-20.3996473741	-1.9889444952	16.0139871937
H	-22.2998906807	-3.5930735357	18.5978715278
H	-20.8864315151	-3.7397777546	19.6373373362
H	-18.6667638870	-2.2605352839	17.4086458286
H	-19.0417464985	-2.2142060161	19.0848753117
C	-16.2809998453	-5.8030000264	12.1999997368
C	-16.6366606864	-5.9909777286	13.6851640567
C	-17.5144925388	-4.8261835520	14.2111528105
C	-17.6631385083	-4.8536863244	15.7231931251
O	-18.6316384403	-5.4345599509	16.2546690815
O	-16.7403893888	-4.3033361170	16.4579776779
H	-15.7499447195	-4.8585806646	12.0413900014
H	-17.1699103414	-6.9406615659	13.8276132687
H	-15.7217220946	-6.0593086874	14.2839687349
H	-17.0567132967	-3.8794793046	13.9131065236
H	-18.5133069843	-4.8883039705	13.7640630920
C	-16.3929999741	-9.8490000770	16.0549998835
C	-16.8432341750	-8.9174080579	17.1796558589
C	-15.9413906337	-7.6997126102	17.3524494328
O	-14.8092749970	-7.6742887864	16.8097947094
O	-16.3770028414	-6.7398376080	18.0802106829
H	-16.4228361096	-9.3352502041	15.0876866256
H	-17.8684841182	-8.5587486638	17.0152351761
H	-16.8559581704	-9.4480050713	18.1437378190
C	-17.5420000290	-9.6659996842	21.8140000041
C	-17.4396055818	-8.2031486635	22.2776084428
C	-18.1115482217	-7.2222207625	21.3258858928
O	-19.3338776940	-7.4018361580	21.0411749094
O	-17.4120460155	-6.2545763928	20.8758902921
H	-18.5894323710	-9.9634370684	21.6954038986
H	-17.9186364932	-8.0978227387	23.2622023744
H	-16.3943427743	-7.9148974889	22.3706576167
C	-14.0159999391	-9.9709998740	25.1559999158
C	-14.6427650965	-8.8824992707	24.2822221836
C	-14.1601717024	-7.4581954665	24.6293224468
C	-14.7325926236	-6.4234069686	23.6673384575
O	-15.4484830142	-5.4764587736	24.1088074063

O	-14.4962094817	-6.5756177503	22.4210700326
H	-14.3859223073	-10.9666265614	24.8798698726
H	-14.4157879375	-9.0755968943	23.2271922081
H	-15.7348672967	-8.9265332294	24.3840256703
H	-14.4409227464	-7.1923527640	25.6547423280
H	-13.0671165122	-7.4084558521	24.5468180029
C	-10.0720000220	-10.4520000153	20.3670000110
C	-11.1706462461	-9.4336765562	20.7215262970
O	-11.3847645113	-8.5092308749	19.6242406371
C	-10.8749850295	-8.6735970644	22.0201092645
H	-10.3146365219	-10.9577831573	19.4266776791
H	-12.1252995832	-9.9681671066	20.8211100480
H	-10.6858850421	-7.8050014843	19.6383200803
H	-11.6817011688	-7.9705123088	22.2522866757
H	-10.7614661799	-9.3689292637	22.8622327206
H	-9.9494030925	-8.0962979139	21.9136292036
C	-9.3519999929	-7.6870000077	26.4129999792
C	-9.7922531440	-6.8874023996	25.1706731961
C	-10.3189329407	-5.4732327952	25.5064678630
C	-10.8888736997	-4.7489806253	24.2826454898
O	-11.7621191476	-5.2821843751	23.5864707827
N	-10.4010593396	-3.5157788422	24.0287820139
H	-8.5368773639	-7.1816792062	26.9475940320
H	-8.9510979161	-6.8019303341	24.4689115520
H	-10.5812560237	-7.4287587640	24.6388019956
H	-11.1376939497	-5.5600672723	26.2350092666
H	-9.5266980889	-4.8785597828	25.9822607635
H	-9.6965769412	-3.1132771155	24.6249309616
H	-10.7227848115	-2.9726513701	23.2193777513
P	-15.4983735358	-2.6936697384	18.9419284251
O	-16.0318546925	-4.0288555833	19.5337815692
O	-14.5849430335	-1.9333321370	19.8937072823
O	-16.5714283832	-1.9279998923	18.1260858765
O	-18.7079643957	-1.4651453136	20.6044192470
Ca	-14.1713855766	-5.5536840797	17.9005482548
Ca	-18.0250603900	-5.1335378858	18.6905621504
Ca	-15.8609816847	-4.5983991116	21.8462694207
Fe	-12.8364862804	-2.1116099193	18.4538884680
Fe	-15.8335762724	-2.4300370749	16.2323668044
O	-14.5131246036	-3.1224436082	17.7040481435
O	-12.4446194059	-4.1417107757	19.2059743671
O	-13.4516829709	-3.9011921126	21.8376759390
O	-17.8697375238	-3.3721660191	22.1617883848
O	-19.6206679461	-4.4951790112	20.6419690646

O	-19.9651101979	-6.6723361411	18.6121244282
O	-13.5844193177	-6.9657890631	19.7871604104
H	-6.9268366441	-6.9913134321	19.7490421216
H	-5.8138093274	-5.7989947848	20.4664802072
H	-7.4866471608	0.8858777202	21.1349686118
H	-6.9093294337	0.2274560350	22.6771163100
H	-8.5805475375	-2.3470867086	16.0345977859
H	-8.1223331929	-0.9846661111	17.0803802107
H	-12.0918283004	3.6804973293	15.6926841649
H	-10.9174681271	2.8465665026	14.6584817412
H	-11.1713579135	-2.7617445378	12.1312409575
H	-12.3021643593	-1.5939111536	11.4155855002
H	-19.1541549993	-0.4469483846	12.4396124897
H	-17.6132305945	0.1101555874	11.7501930492
H	-21.3233043749	-3.9892818486	11.5900604606
H	-22.9870433833	-3.5024072088	11.9662866702
H	-15.6420536109	-6.6179057289	11.8381186378
H	-17.1855960778	-5.7858391511	11.5767443850
H	-15.3614758546	-10.1738518895	16.2173173894
H	-17.0364229558	-10.7357341002	15.9927455031
H	-17.0359441669	-9.8049919965	20.8508287102
H	-17.0690976046	-10.3369684690	22.5402459319
H	-12.9227291261	-9.9811842488	25.0528245347
H	-14.2458660639	-9.8126353745	26.2184433668
H	-9.1096121177	-9.9400592079	20.2447590550
H	-9.9678467601	-11.2057908363	21.1578092308
H	-10.1855069773	-7.8130302131	27.1159283477
H	-8.9987194397	-8.6847012876	26.1281687616
H	-19.8388480225	-7.1124258987	19.4999431314
H	-19.8760936578	-7.3415769798	17.9237064889
H	-18.9838645447	-4.0603722928	21.3308590260
H	-19.7523931516	-5.4138848345	20.9449286741
H	-18.3252219855	-2.1297810383	21.2622769897
H	-18.2235825050	-3.1822597811	23.0389784729
H	-13.0138543403	-3.0232407245	21.7869914732
H	-12.8658535586	-4.4474309592	22.4149497298
H	-11.3906927034	-4.3370923839	19.2396084686
H	-12.7438142085	-4.1814731506	20.1445747641
H	-12.7930460187	-7.5630098064	19.7464034083
H	-13.8541198299	-6.9383061749	20.7244144290
C	-17.9723277934	-0.2530414119	20.6509234172
H	-18.2855128923	0.3725445768	21.5023284658
H	-16.8905127719	-0.4234594044	20.7164833705
H	-18.1627342321	0.3058201235	19.7286645616

Int_{OH}

Energy with the medium-sized basis set:	-5387.35547
Solution energy with the medium-sized basis set:	-5387.44236
Energy with larger basis sets:	-5389.37452
Zero-point energy:	1.55245
Dispersion effect:	-0.31611

C	-6.8650001839	-6.1059999021	20.3889999027
C	-7.7296896042	-4.9534566437	19.8684317828
C	-9.2134059328	-5.3177881591	19.6533997266
O	-9.5430567897	-6.5191399718	19.7501440043
O	-9.9629970048	-4.3197301044	19.3761248640
H	-7.2116250457	-6.4408984461	21.3731817630
H	-7.6906907689	-4.0939860841	20.5517834969
H	-7.3426709833	-4.5863645670	18.9059855757
C	-7.4140001730	-0.0290000743	21.7369999314
C	-8.7931304613	-0.6464116224	22.0111475196
C	-9.4927290918	-1.0003743562	20.6943415151
C	-10.9462180218	-1.4356992828	20.7913956899
O	-11.4042947926	-1.9715294576	21.8183524204
O	-11.6189992873	-1.1934507762	19.7163096258
H	-6.7813677603	-0.7201629241	21.1654307018
H	-8.6859782751	-1.5468169166	22.6297126184
H	-9.4120810179	0.0567916186	22.5850451106
H	-9.4476834506	-0.1479254894	20.0057699848
H	-8.9698189652	-1.8305188394	20.1969559641
C	-8.8830001017	-1.7600000189	16.9099999906
C	-10.2385493877	-1.0795766807	16.7489749273
S	-11.5670204820	-2.3404091340	16.5401061417
H	-8.9006983248	-2.4570414129	17.7538198829
H	-10.4733476509	-0.4654417154	17.6210744784
H	-10.2496707145	-0.4417313259	15.8587994079
C	-11.9690000170	2.8629998231	14.9700001680
C	-12.3931435412	1.5443961842	15.6357613178
C	-13.8631264316	1.5185576865	16.1227315247
C	-14.1925580303	0.1653786470	16.7556843315
O	-13.5394395466	-0.1676884024	17.7733390945
O	-15.0945539553	-0.5318394585	16.1700313218
H	-12.5799886009	3.0791812200	14.0839249253
H	-12.2423223407	0.7160607340	14.9297079019
H	-11.7491487560	1.3432505164	16.4978563645
H	-14.0100949543	2.3003396405	16.8804847507
H	-14.5522114961	1.7095511607	15.2935494699

C	-12.1639999270	-2.3060000188	12.2389999991
C	-13.3334358618	-3.3021512397	12.3086504061
C	-13.1956512104	-4.3206855452	13.4581798231
C	-13.9259308035	-4.0410028649	14.7777656163
O	-14.7426878426	-3.0345592729	14.8158282903
O	-13.7078371812	-4.8365434496	15.7095444270
H	-12.0762861961	-1.7474448277	13.1784199672
H	-14.2761625512	-2.7549520458	12.4258554923
H	-13.3966816359	-3.8430183827	11.3536488311
H	-13.5521211654	-5.3103964586	13.1431533638
H	-12.1409871384	-4.4652851316	13.7255566579
C	-18.0649999001	-0.5230001845	12.5230003354
C	-17.3843214766	-0.1896647676	13.8576648296
C	-18.1969535883	-0.8336259125	14.9664750186
O	-19.3937251120	-0.5160897681	15.0923435700
O	-17.6439141233	-1.7504536658	15.6951526087
H	-18.0709948380	-1.6054687744	12.3454102480
H	-16.3502380314	-0.5389730616	13.8832131998
H	-17.3785784674	0.8966503936	14.0138841227
C	-21.9319999276	-3.3249999991	12.2140002005
C	-21.5669856116	-3.4325740894	13.7071728197
C	-22.5351092174	-2.6474016527	14.6149725472
C	-22.2985218366	-2.8457596452	16.1226193817
N	-21.0421422537	-2.2298234775	16.5577123430
C	-20.5707740123	-2.3084874215	17.8042296446
N	-21.1814752521	-3.0127461007	18.7766372153
N	-19.4636364600	-1.6210543719	18.1378684397
H	-21.8937096129	-2.2825876986	11.8730622092
H	-21.5680251616	-4.4892440462	14.0113356008
H	-20.5441628436	-3.0676117125	13.8628375846
H	-22.4798035157	-1.5751521018	14.3786409638
H	-23.5664694766	-2.9617210902	14.3991292724
H	-23.1378478538	-2.4127646995	16.6874905538
H	-22.2795355565	-3.9242399018	16.3400097693
H	-20.5163040508	-1.6061292166	15.9223126375
H	-21.8089325943	-3.7492835440	18.4887142505
H	-20.5059373981	-3.2531197673	19.5506203375
H	-18.8211085579	-1.3761067761	17.3905359029
H	-19.0157905557	-1.9061000032	19.0043432633
C	-16.2809998394	-5.8030000367	12.1999997235
C	-16.6518048086	-5.9572042351	13.6895468463
C	-17.5073517024	-4.7682692248	14.2079338716
C	-17.6770466348	-4.7878827339	15.7210124935
O	-18.6587836227	-5.3468637366	16.2523976613

O	-16.7543551254	-4.2472972960	16.4618920287
H	-15.7297988241	-4.8729060888	12.0252601673
H	-17.2070829362	-6.8926971774	13.8399603499
H	-15.7411367140	-6.0401858141	14.2932561794
H	-17.0185449310	-3.8334866316	13.9183811475
H	-18.5012106301	-4.8026579540	13.7471575458
C	-16.3929999693	-9.8490000849	16.0549998686
C	-16.9862732424	-8.7560356874	16.9458058616
C	-16.0041962387	-7.6418917584	17.2909298415
O	-14.8448600545	-7.6410692325	16.8082131676
O	-16.4183393795	-6.7154778354	18.0764538871
H	-16.0356240143	-9.4292369063	15.1093185956
H	-17.8518770038	-8.2801830277	16.4611837364
H	-17.3637762138	-9.1666126616	17.8924820822
C	-17.5420000144	-9.6659995898	21.8139999780
C	-17.3290930047	-8.1706992390	22.0635392516
C	-18.0516334733	-7.2547386953	21.0824133190
O	-19.0107671382	-7.7195176831	20.4211064778
O	-17.6310051147	-6.0380709362	20.9983034594
H	-18.6060784553	-9.9217178365	21.8372761189
H	-17.6692867420	-7.8970465160	23.0750034915
H	-16.2658173613	-7.9208213833	22.0252181758
C	-14.0159999338	-9.9709998898	25.1559999205
C	-14.6148144237	-8.8879647161	24.2611295437
C	-14.1582029113	-7.4666338805	24.6459726615
C	-14.7181774419	-6.4378708935	23.6791959844
O	-15.4561876927	-5.5015478577	24.1050845530
O	-14.4541237096	-6.5867360163	22.4359677664
H	-14.3587207154	-10.9707151440	24.8603784700
H	-14.3387625442	-9.0692978623	23.2161332594
H	-15.7102710917	-8.9401396380	24.3106355987
H	-14.4747963127	-7.2172724900	25.6647997926
H	-13.0637960264	-7.4027349163	24.5982476688
C	-10.0720000130	-10.4520000283	20.3670000107
C	-11.1608454486	-9.4233791366	20.7143657438
O	-11.3524076490	-8.4980353659	19.6131315298
C	-10.8681655097	-8.6679159652	22.0165956202
H	-10.3128298047	-10.9522093887	19.4233464029
H	-12.1224321772	-9.9468602333	20.8046885638
H	-10.6631633850	-7.7857048227	19.6496992889
H	-11.6720020440	-7.9610423192	22.2476212991
H	-10.7646314093	-9.3670614538	22.8566593494
H	-9.9382227312	-8.0964830560	21.9178540451
C	-9.3519999998	-7.6869999961	26.4129999709

C	-9.7683537588	-6.8613720303	25.1813297083
C	-10.2978784156	-5.4542271017	25.5407591469
C	-10.8727810869	-4.7200522392	24.3276005209
O	-11.7583478497	-5.2468657095	23.6413480102
N	-10.3763830002	-3.4921839054	24.0682784765
H	-8.5511044126	-7.1911972088	26.9771460017
H	-8.9154753376	-6.7617500195	24.4957420947
H	-10.5497609314	-7.3889120188	24.6248004234
H	-11.1152964614	-5.5546818988	26.2687663024
H	-9.5068291620	-4.8636787707	26.0232911761
H	-9.6617680956	-3.0967852982	24.6570880535
H	-10.7054532234	-2.9434020063	23.2657536673
P	-15.4498227800	-2.7766023077	19.0180499752
O	-15.7684580676	-4.2209125173	19.5141366711
O	-14.6019285251	-1.9647630147	19.9855458501
O	-16.6765503166	-2.1332853871	18.3288578578
Ca	-14.1830299546	-5.5481818176	17.9701170894
Ca	-17.9446622527	-5.0102818602	18.7139746157
Ca	-15.7770469631	-4.6301277982	21.8502808613
Fe	-12.8326689236	-2.0438139505	18.4976812226
Fe	-15.8701067655	-2.3716999368	16.3292081060
O	-14.4881341628	-3.0178379120	17.7202878373
O	-12.4382089025	-4.0929647877	19.2302761799
O	-13.3970483520	-3.8988362598	21.8818157662
O	-17.1759425544	-2.6484982602	21.8704409828
O	-19.0222217767	-3.5027662943	20.3020069431
O	-20.1199112123	-6.2004555143	18.6387203511
O	-13.5408111930	-6.9756802856	19.8117121511
H	-6.9285698748	-6.9667002916	19.7163074185
H	-5.8127818192	-5.8056822023	20.4781455822
H	-7.5088270013	0.8943693639	21.1514503521
H	-6.8855089262	0.2173629533	22.6666680488
H	-8.6191961529	-2.3312403205	16.0119994998
H	-8.0948655954	-1.0130597314	17.0824322415
H	-12.0749927448	3.7089038801	15.6618904111
H	-10.9204926419	2.8193634449	14.6514898248
H	-11.2129753499	-2.8284344361	12.0739270506
H	-12.3002299340	-1.5845058376	11.4235213541
H	-19.1012887966	-0.1727438578	12.5293842101
H	-17.5428860481	-0.0516782430	11.6815533317
H	-21.2373158385	-3.9047474558	11.5954887777
H	-22.9457806556	-3.7023564274	12.0253105892
H	-15.6558860145	-6.6386531764	11.8629501241
H	-17.1801580833	-5.7812248755	11.5693564436

H	-15.5347864127	-10.3237865143	16.5412321945
H	-17.1381174445	-10.6235410268	15.8326846453
H	-17.1570538415	-9.9530427941	20.8288701900
H	-17.0202112800	-10.2648739904	22.5698380306
H	-12.9190455499	-9.9662351612	25.1025727625
H	-14.2953681233	-9.8209700509	26.2077192590
H	-9.1025922825	-9.9513255089	20.2539576157
H	-9.9825378375	-11.2095126318	21.1560047620
H	-10.2001033288	-7.8325745166	27.0942242776
H	-8.9879263446	-8.6765110336	26.1136683328
H	-19.8223583725	-6.8688896926	19.3337702845
H	-20.1017506327	-6.6513010533	17.7841967469
H	-17.9574481198	-2.8453455682	21.2244069860
H	-19.3136175083	-4.1323121685	20.9776230652
H	-16.7573417838	-1.8291980965	21.5733095367
H	-12.9803651646	-3.0103010721	21.8418845615
H	-12.8050869870	-4.4343290262	22.4651813803
H	-11.3883244756	-4.2880891759	19.2547124954
H	-12.7278604765	-4.1416848806	20.1723716770
H	-12.7524053269	-7.5765149243	19.7442585464
H	-13.7720655225	-6.9380301196	20.7581801386

TS_{OH}

Energy with the medium-sized basis set:	-5387.33045
Solution energy with the medium-sized basis set:	-5387.41598
Energy with larger basis sets:	-5389.35038
Zero-point energy:	2.00113
Imaginary frequency:	-56.6641
Dispersion effect:	-0.31790

C	-6.8650000000	-6.1060000000	20.3890000000
C	-7.7185430000	-4.9095050000	19.9631070000
C	-9.2013240000	-5.2417680000	19.7055230000
O	-9.5607790000	-6.4370770000	19.7686060000
O	-9.9226650000	-4.2233990000	19.4371680000
H	-7.2264560000	-6.5280580000	21.3335030000
H	-7.6837170000	-4.1119710000	20.7185280000
H	-7.3220560000	-4.4613470000	19.0404180000
C	-7.4140000000	-0.0290000000	21.7370000000
C	-8.7655650000	-0.7139330000	21.9778690000
C	-9.5366640000	-0.8491840000	20.6640280000
C	-10.9597320000	-1.3808580000	20.7451110000
O	-11.3906240000	-1.9548920000	21.7657180000
O	-11.6292310000	-1.1671380000	19.6700140000

H	-6.8102570000	-0.5969320000	21.0179010000
H	-8.6053820000	-1.7081610000	22.4147820000
H	-9.3576410000	-0.1404300000	22.7038310000
H	-9.5801280000	0.1208420000	20.1515610000
H	-9.0038300000	-1.5315410000	19.9874100000
C	-8.8830000000	-1.7600000000	16.9100000000
C	-10.2549080000	-1.1038320000	16.7585490000
S	-11.5874540000	-2.3689980000	16.5527480000
H	-8.8861500000	-2.4595430000	17.7521580000
H	-10.4889100000	-0.4960430000	17.6346410000
H	-10.2764920000	-0.4607260000	15.8721670000
C	-11.9690000000	2.8630000000	14.9700000000
C	-12.3998600000	1.5455440000	15.6393420000
C	-13.8953260000	1.4802730000	16.0334760000
C	-14.2276860000	0.1553820000	16.7291870000
O	-13.5493450000	-0.1477080000	17.7382840000
O	-15.1702900000	-0.5425490000	16.2156370000
H	-12.5287810000	3.0452840000	14.0433500000
H	-12.1796130000	0.7066840000	14.9652620000
H	-11.8059470000	1.3804640000	16.5440270000
H	-14.1237010000	2.2980240000	16.7322850000
H	-14.5379360000	1.5974170000	15.1545020000
C	-12.1640000000	-2.3060000000	12.2390000000
C	-13.3774590000	-3.2434130000	12.3427850000
C	-13.2350990000	-4.2875750000	13.4677960000
C	-13.9469880000	-4.0284760000	14.8007920000
O	-14.7923440000	-3.0536400000	14.8644510000
O	-13.6870940000	-4.8228110000	15.7240500000
H	-12.0038990000	-1.7773400000	13.1862310000
H	-14.2848390000	-2.6536020000	12.5160720000
H	-13.5119530000	-3.7588010000	11.3812330000
H	-13.6018910000	-5.2678690000	13.1355660000
H	-12.1795290000	-4.4443000000	13.7216030000
C	-18.0650000000	-0.5230000000	12.5230000000
C	-17.3226540000	-0.7675630000	13.8255710000
C	-18.2473930000	-1.3122470000	14.8941680000
O	-19.4845850000	-1.1972020000	14.7703650000
O	-17.7089020000	-1.8743070000	15.9224090000
H	-18.4792710000	-1.4558500000	12.1234250000
H	-16.4818250000	-1.4584310000	13.6952970000
H	-16.8756560000	0.1564700000	14.2168450000
C	-21.9320000000	-3.3250000000	12.2140000000
C	-21.5693140000	-3.6470080000	13.6720680000
C	-22.5758290000	-3.0489030000	14.6741030000

C	-22.2371990000	-3.3247920000	16.1481970000
N	-21.0571950000	-2.5624030000	16.5687920000
C	-20.6017870000	-2.5277520000	17.8177040000
N	-21.2440580000	-3.1697380000	18.8296660000
N	-19.5266050000	-1.7738380000	18.0991300000
H	-21.9263110000	-2.2416790000	12.0417220000
H	-21.5253880000	-4.7364020000	13.8150540000
H	-20.5678160000	-3.2571940000	13.8832320000
H	-22.6472780000	-1.9628550000	14.5238270000
H	-23.5749090000	-3.4624010000	14.4750290000
H	-23.0867800000	-3.0422440000	16.7849370000
H	-22.0636310000	-4.4037480000	16.2837570000
H	-20.4497300000	-2.0954420000	15.8612890000
H	-21.7100590000	-4.0293500000	18.5706830000
H	-20.6452400000	-3.2988370000	19.6481950000
H	-18.8782370000	-1.5894080000	17.3247130000
H	-19.0311820000	-1.9742220000	18.9575990000
C	-16.2810000000	-5.8030000000	12.2000000000
C	-16.6281760000	-6.0007580000	13.6881170000
C	-17.5038200000	-4.8432450000	14.2375240000
C	-17.6588540000	-4.8992590000	15.7471470000
O	-18.6580240000	-5.4429820000	16.2730910000
O	-16.7136650000	-4.4119270000	16.4892490000
H	-15.7611180000	-4.8524770000	12.0406100000
H	-17.1590570000	-6.9524410000	13.8249670000
H	-15.7095340000	-6.0705870000	14.2812910000
H	-17.0258410000	-3.8967750000	13.9705350000
H	-18.4982100000	-4.8824810000	13.7794700000
C	-16.3930000000	-9.8490000000	16.0550000000
C	-16.2905100000	-9.3196260000	17.4966780000
C	-15.7090910000	-7.9088950000	17.5551790000
O	-14.5993990000	-7.6919120000	17.0073470000
O	-16.3697840000	-7.0048140000	18.1745920000
H	-17.0830950000	-9.2381670000	15.4597330000
H	-17.2652720000	-9.3305200000	17.9952340000
H	-15.6141830000	-9.9696470000	18.0695650000
C	-17.5420000000	-9.6660000000	21.8140000000
C	-17.2485780000	-8.1765150000	22.0177360000
C	-18.0938460000	-7.2297520000	21.1797130000
O	-19.1391490000	-7.6507570000	20.6390950000
O	-17.6724840000	-6.0046460000	21.0793370000
H	-18.5934680000	-9.8933260000	22.0163780000
H	-17.4036630000	-7.8918570000	23.0697120000
H	-16.1970750000	-7.9580070000	21.8086090000

C	-14.0160000000	-9.9710000000	25.1560000000
C	-14.6587660000	-8.8810540000	24.3107010000
C	-14.3115430000	-7.4580390000	24.7886940000
C	-14.7835830000	-6.4409080000	23.7696470000
O	-15.5817970000	-5.5146230000	24.1079420000
O	-14.3834080000	-6.5982500000	22.5660120000
H	-14.2906840000	-10.9716020000	24.7987330000
H	-14.3363270000	-8.9783250000	23.2686330000
H	-15.7490420000	-9.0079440000	24.3186350000
H	-14.7612920000	-7.2451460000	25.7641890000
H	-13.2223040000	-7.3522890000	24.8774390000
C	-10.0720000000	-10.4520000000	20.3670000000
C	-11.1292950000	-9.3965580000	20.7292400000
O	-11.3225050000	-8.4713190000	19.6260020000
C	-10.7967110000	-8.6469510000	22.0247790000
H	-10.3377300000	-10.9423710000	19.4249420000
H	-12.0978590000	-9.9028820000	20.8434450000
H	-10.6439010000	-7.7499910000	19.6620880000
H	-11.5919970000	-7.9402070000	22.2833160000
H	-10.6698480000	-9.3474770000	22.8601850000
H	-9.8699750000	-8.0765280000	21.8977140000
C	-9.3520000000	-7.6870000000	26.4130000000
C	-9.8322420000	-6.8981900000	25.1841400000
C	-10.0308900000	-5.3941700000	25.4636670000
C	-10.7195990000	-4.6741830000	24.3033180000
O	-11.7220370000	-5.1700420000	23.7721030000
N	-10.1995400000	-3.4875100000	23.9310390000
H	-8.3879070000	-7.3123460000	26.7816020000
H	-9.1172330000	-7.0207490000	24.3597740000
H	-10.7832230000	-7.3055100000	24.8260480000
H	-10.6800490000	-5.2756660000	26.3440620000
H	-9.0706810000	-4.9199230000	25.7090220000
H	-9.3688080000	-3.1355740000	24.3774610000
H	-10.5990000000	-2.9439230000	23.1562920000
P	-15.5309780000	-2.8214310000	19.2668020000
O	-15.6335440000	-4.3814400000	19.5133120000
O	-14.4451970000	-1.9842470000	19.9704180000
O	-16.7379120000	-2.2713640000	18.4403740000
Ca	-14.0849930000	-5.5025480000	17.9757890000
Ca	-17.7544220000	-5.1689620000	18.6287280000
Ca	-15.6253360000	-4.7076780000	21.8279930000
Fe	-12.9103090000	-2.0331890000	18.4910450000
Fe	-15.8294150000	-2.4301510000	16.4921810000
O	-14.5500120000	-3.0161380000	17.8052290000

O	-12.3936030000	-4.0962370000	19.2353740000
O	-13.3309260000	-3.8853680000	21.9598460000
O	-16.6234970000	-2.6706520000	21.0170360000
O	-18.8985700000	-3.6672050000	20.4065030000
O	-20.0564890000	-6.1000240000	18.7785540000
O	-13.5454650000	-6.9981850000	19.8631640000
H	-6.9188630000	-6.9031190000	19.6409050000
H	-5.8133210000	-5.8192690000	20.5202910000
H	-7.5532400000	0.9798970000	21.3281400000
H	-6.8319690000	0.0638120000	22.6627130000
H	-8.6140190000	-2.3249380000	16.0094560000
H	-8.1087420000	-0.9981380000	17.0802930000
H	-12.1379530000	3.7199110000	15.6352820000
H	-10.9021910000	2.8386280000	14.7177970000
H	-11.2495430000	-2.8708000000	12.0162480000
H	-12.3001180000	-1.5578280000	11.4475790000
H	-18.9020430000	0.1646570000	12.6728950000
H	-17.3988300000	-0.0981050000	11.7617450000
H	-21.2140940000	-3.7766330000	11.5198120000
H	-22.9308590000	-3.7022760000	11.9560740000
H	-15.6348690000	-6.6106080000	11.8356690000
H	-17.1883250000	-5.7945880000	11.5811660000
H	-15.4112170000	-9.8161560000	15.5738150000
H	-16.7580040000	-10.8830410000	16.0391440000
H	-17.3331200000	-9.9641660000	20.7808180000
H	-16.9174710000	-10.2753340000	22.4769520000
H	-12.9206980000	-9.8982970000	25.1275670000
H	-14.3225810000	-9.9002210000	26.2085330000
H	-9.0906750000	-9.9778760000	20.2434420000
H	-9.9944420000	-11.2137710000	21.1531150000
H	-10.0745640000	-7.6140220000	27.2361330000
H	-9.2262620000	-8.7485050000	26.1706470000
H	-19.8574500000	-6.7517180000	19.5237240000
H	-20.1332170000	-6.6136620000	17.9631160000
H	-18.0929970000	-3.1169080000	20.7019860000
H	-18.8643480000	-4.4608140000	20.9748290000
H	-16.4452840000	-1.7754580000	21.3320110000
H	-12.9209940000	-2.9997530000	21.8335860000
H	-12.7209850000	-4.3727200000	22.5664280000
H	-11.3329270000	-4.2190850000	19.2551480000
H	-12.6622620000	-4.1368130000	20.1793000000
H	-12.7477490000	-7.5820410000	19.7573340000
H	-13.6735620000	-6.9115170000	20.8231930000

Prod

Energy with the medium-sized basis set:	-5387.33350
Solution energy with the medium-sized basis set:	-5387.42106
Energy with larger basis sets:	-5389.35171
Zero-point energy:	1.55529
Dispersion effect:	-0.32444

C	-6.8650001973	-6.1059998854	20.3889998922
C	-7.6895045971	-5.0222934457	19.6889351253
C	-9.1829929336	-5.3733660355	19.5220909470
O	-9.5239076810	-6.5653336737	19.7117824375
O	-9.9185614057	-4.3916664945	19.1837857191
H	-7.2181641482	-6.2645137624	21.4148962164
H	-7.6260688767	-4.0660482829	20.2247360739
H	-7.2893826071	-4.8276937960	18.6821911273
C	-7.4140002595	-0.0290001164	21.7369998977
C	-8.7554625925	-0.7642722779	21.9087714376
C	-9.5631496528	-0.7771582783	20.6057465656
C	-10.9472472073	-1.4306180437	20.6512508917
O	-11.3227223251	-2.0549210389	21.6741892266
O	-11.6291888247	-1.2573030268	19.5862855460
H	-6.8029925076	-0.5066446046	20.9605952189
H	-8.5689806863	-1.7980642974	22.2284529491
H	-9.3457012979	-0.2896992888	22.7049907885
H	-9.7017831751	0.2481059057	20.2345712079
H	-9.0015461874	-1.3074643078	19.8245027811
C	-8.8830001358	-1.7600000206	16.9099999943
C	-10.1939326535	-0.9937487550	16.7554209631
S	-11.5888922957	-2.1478533551	16.4154498064
H	-8.9675925570	-2.5114386111	17.7021905904
H	-10.4270625916	-0.4375884124	17.6661875042
H	-10.1317632751	-0.2886642046	15.9184521089
C	-11.9690000425	2.8629997823	14.9700001871
C	-12.4065183929	1.5564388588	15.6403612008
C	-13.8960906516	1.5311543883	16.0621372717
C	-14.2205755694	0.1624038594	16.6561998068
O	-13.6809270683	-0.1283463410	17.7495981913
O	-14.9765416113	-0.5955954686	15.9497103624
H	-12.5414970419	3.0538724690	14.0524690952
H	-12.2193756884	0.7138215551	14.9616087449
H	-11.8003376006	1.3753596353	16.5337515038
H	-14.0763374863	2.3034434940	16.8214482825
H	-14.5461672826	1.7266316800	15.2023516884

C	-12.1639999249	-2.3060000196	12.2389999973
C	-13.0854793303	-3.5273701968	12.0944938609
C	-12.9617551677	-4.5335240743	13.2528642348
C	-13.7177475390	-4.2322817374	14.5527735800
O	-14.5600697198	-3.2404221552	14.5317737761
O	-13.5132867555	-4.9863635455	15.5186884200
H	-12.3719667900	-1.7748621636	13.1740877707
H	-14.1261879995	-3.1897334916	12.0194773106
H	-12.8516935075	-4.0468739843	11.1533936451
H	-13.3128195699	-5.5253285162	12.9343755946
H	-11.9097145641	-4.6709807747	13.5345167302
C	-18.0649998185	-0.5230001821	12.5230003828
C	-17.2354614945	-0.8399662758	13.7586266180
C	-18.0725894634	-1.4353955048	14.8777140490
O	-19.3202465041	-1.3680935445	14.8231400960
O	-17.4469057238	-1.9909771782	15.8591852994
H	-18.5183733770	-1.4300829316	12.1072751963
H	-16.4113097818	-1.5261340739	13.5248532010
H	-16.7476549626	0.0579888820	14.1596060958
C	-21.9319999157	-3.3250000140	12.2140003223
C	-21.6986228320	-3.6644095511	13.6951722969
C	-22.6314102974	-2.8711408061	14.6317988687
C	-22.3926719580	-3.1352676260	16.1286504168
N	-21.0702599865	-2.6429172871	16.5251292845
C	-20.5558856303	-2.7337091740	17.7460503836
N	-21.2869307030	-3.1154364200	18.8238156421
N	-19.2676859237	-2.4244048245	17.9236072868
H	-21.7309652198	-2.2638935923	12.0229260152
H	-21.8489082810	-4.7410753443	13.8619759275
H	-20.6547674151	-3.4478670619	13.9484837475
H	-22.5127668567	-1.7952951044	14.4415664858
H	-23.6781491309	-3.1185730599	14.4053867555
H	-23.1714292828	-2.6296788912	16.7190152612
H	-22.4675161015	-4.2149316245	16.3298495982
H	-20.4433375583	-2.1970089360	15.8197455618
H	-22.1375630802	-3.6274050726	18.6484301942
H	-20.7369608392	-3.4562682963	19.6116703804
H	-18.6562290395	-2.1665216609	17.1288556695
H	-18.8840115273	-2.1836825822	18.8291816402
C	-16.2809997967	-5.8030000418	12.1999996476
C	-16.5964721665	-6.0341057330	13.6850711653
C	-17.4195389851	-4.8538383424	14.2553852429
C	-17.5151332560	-4.8768187199	15.7663171124
O	-18.5438253360	-5.3193902460	16.3291476134

O	-16.5055495172	-4.4479659017	16.4651303573
H	-15.7048246989	-4.8822043364	12.0640290244
H	-17.1573685229	-6.9697547121	13.8139329689
H	-15.6697199378	-6.1454808226	14.2579727975
H	-16.9298408481	-3.9257900758	13.9487689347
H	-18.4332119317	-4.8713523494	13.8401927772
C	-16.3929999575	-9.8490000893	16.0549998596
C	-16.8172119376	-8.9825478306	17.2506889859
C	-15.9864149053	-7.7107088157	17.4529072657
O	-14.8974748453	-7.5705790079	16.8467422581
O	-16.4454114771	-6.8334055731	18.2718505595
H	-16.5108741473	-9.3004469929	15.1140264398
H	-17.8707820214	-8.6839908955	17.1655233753
H	-16.7451754308	-9.5591479788	18.1854111063
C	-17.5420000190	-9.6659995011	21.8139999616
C	-17.1788401679	-8.1955323751	22.0603998144
C	-18.0516359647	-7.1757720493	21.3379460916
O	-19.1522242979	-7.5226738620	20.8677839633
O	-17.5869357127	-5.9592512787	21.2735032439
H	-18.5837290662	-9.8642319494	22.0853323995
H	-17.2448735869	-7.9640561122	23.1344157376
H	-16.1363183874	-8.0045093986	21.7835862964
C	-14.0159999494	-9.9709999062	25.1559998960
C	-14.7410613491	-8.7666926317	24.5955631109
C	-13.9556396146	-7.4580925329	24.8244282831
C	-14.4459141458	-6.4572345646	23.8112990523
O	-15.1738762541	-5.4825437116	24.1734277485
O	-14.1882992780	-6.7173425523	22.5837870630
H	-14.5795211921	-10.8996157014	24.9953251486
H	-14.8676504938	-8.9031225103	23.5177760421
H	-15.7447492642	-8.6781947097	25.0338956948
H	-14.0880314180	-7.0830026134	25.8440248308
H	-12.8897492816	-7.6328636554	24.6441851199
C	-10.0720000013	-10.4520000464	20.3670000132
C	-11.1605658516	-9.4117624458	20.6841683408
O	-11.3423129645	-8.5084061852	19.5632506386
C	-10.8682679170	-8.6362330528	21.9748655985
H	-10.3051688808	-10.9708046374	19.4312345388
H	-12.1240281605	-9.9314823411	20.7806844134
H	-10.6529372463	-7.7905801206	19.5944517263
H	-11.6833020328	-7.9454459567	22.2127607488
H	-10.7383424065	-9.3261830536	22.8193910611
H	-9.9518174008	-8.0476312224	21.8567493872
C	-9.3519999918	-7.6869999894	26.4129999684

C	-9.7039248948	-6.8843421756	25.1479721493
C	-10.0509718847	-5.4068909852	25.4353004322
C	-10.6665654524	-4.7093456714	24.2199526230
O	-11.6026299279	-5.2458164082	23.6113841125
N	-10.1643207446	-3.5056867615	23.8814805374
H	-8.4828286945	-7.2617412495	26.9320310622
H	-8.8695526441	-6.9272624341	24.4346730211
H	-10.5611367650	-7.3409872510	24.6434025455
H	-10.8028242627	-5.3653760850	26.2372460927
H	-9.1652844655	-4.8674268471	25.7982851350
H	-9.3887694012	-3.1166637886	24.3924356328
H	-10.5312907808	-2.9776729647	23.0777488445
P	-15.7313148849	-2.6700083293	19.7671036666
O	-15.6200627886	-4.2343006134	19.6480641966
O	-14.4404995902	-1.9042871897	19.9498058249
O	-16.8725780115	-2.1848172545	18.9066727246
Ca	-14.1858111054	-5.4157446143	17.8609793120
Ca	-17.7382598373	-4.8877597459	18.6315266535
Ca	-15.4636992986	-4.8818171331	21.8849381122
Fe	-12.9793986118	-2.0636221410	18.3430554639
Fe	-15.4527142100	-2.5381603350	16.1578939960
O	-14.3512491286	-3.0078097840	17.4547690220
O	-12.4105244904	-4.1240065954	19.0927052173
O	-13.2058030496	-3.9749532802	21.8333439747
O	-16.3690853038	-2.6561126386	21.4078451899
O	-18.9589798533	-3.7537628819	20.6924219407
O	-19.9148446086	-6.0125886164	18.8964811924
O	-13.5243860088	-6.9702112910	19.7249884016
H	-6.9671618671	-7.0602146671	19.8635721482
H	-5.8011438530	-5.8367355342	20.4307110496
H	-7.5731388025	1.0150959163	21.4377430950
H	-6.8317549371	-0.0260967677	22.6673141966
H	-8.6232484755	-2.2856746646	15.9828063071
H	-8.0575494886	-1.0737675122	17.1529618049
H	-12.1161137183	3.7226610316	15.6377248699
H	-10.9065180050	2.8281324529	14.6991283015
H	-11.1094609961	-2.6102387545	12.2597755977
H	-12.2984541037	-1.6054046017	11.4047741366
H	-18.8804544059	0.1649198604	12.7657898395
H	-17.4462487786	-0.0653253754	11.7412386472
H	-21.2702145806	-3.9115461521	11.5667724415
H	-22.9674219905	-3.5330821256	11.9124519596
H	-15.6980678780	-6.6325097616	11.7813156320
H	-17.2031181821	-5.7121901692	11.6097720584

H	-15.3389110877	-10.1285643877	16.1386544307
H	-16.9980417948	-10.7624305987	16.0006923994
H	-17.4202518982	-9.9242603440	20.7564610732
H	-16.8933018214	-10.3237049204	22.4034115964
H	-13.0366052263	-10.0914628118	24.6760107254
H	-13.8424694690	-9.8769144365	26.2371269829
H	-9.1004474081	-9.9559677573	20.2523718387
H	-9.9922489969	-11.1933045421	21.1724336434
H	-10.1918227343	-7.6950665362	27.1197852615
H	-9.1149547196	-8.7271133875	26.1613139004
H	-19.7532822069	-6.6321985905	19.6734395644
H	-19.9880709724	-6.5636806517	18.1058998112
H	-18.3288896458	-3.1025168981	21.0540667084
H	-18.7113809957	-4.6030544079	21.1369642401
H	-16.0715880074	-1.8349359661	21.8259171075
H	-12.7584030843	-3.0981124172	21.7245977387
H	-12.5872320554	-4.4903434233	22.4105761271
H	-11.3759001909	-4.3076655081	19.0758764705
H	-12.6466084626	-4.1701474833	20.0445573133
H	-12.7431983508	-7.5775407806	19.6037154226
H	-13.6059258104	-6.9060661977	20.6903393596

React_{pnp}

Energy with the medium-sized basis set:	-5899.32545
Solution energy with the medium-sized basis set:	-5899.41409
Energy with larger basis sets:	-5901.51452
Zero-point energy:	1.66439
Dispersion effect:	-0.35320

C	-6.8650001776	-6.1059999006	20.3889998990
C	-7.5955319782	-5.1079691456	19.4868977672
C	-9.0974854791	-5.4165961972	19.3534817311
O	-9.4392398484	-6.6229483126	19.3723624492
O	-9.8448810482	-4.3958168256	19.2110587832
H	-7.2414938404	-6.0532076899	21.4185968827
H	-7.4804766706	-4.0803241310	19.8493044985
H	-7.1640041317	-5.1342067222	18.4742239959
C	-7.4140000740	-0.0290000323	21.7369999787
C	-8.7825137028	-0.7100216903	21.9294790114
C	-9.5373796290	-0.8603574311	20.6018373758
C	-10.9306794600	-1.4899482587	20.6647448078
O	-11.3202608135	-2.0608181143	21.7166062951
O	-11.6075938038	-1.3721588206	19.5916318364

H	-6.7812642215	-0.6088114941	21.0529777352
H	-8.6388074786	-1.7017901966	22.3779105390
H	-9.3923896107	-0.1312881034	22.6371256883
H	-9.6416297841	0.1161849328	20.1096332332
H	-8.9569177418	-1.4877051527	19.9108224671
C	-8.8830000600	-1.7599999994	16.9099999804
C	-10.2348305204	-1.0816052743	16.7198093473
S	-11.5532812206	-2.3307700387	16.4142679288
H	-8.9298360569	-2.4891685836	17.7250588437
H	-10.5075418890	-0.5060916814	17.6070434442
H	-10.2083832464	-0.4070060942	15.8571814957
C	-11.9689999928	2.8629998959	14.9700000929
C	-12.3508366826	1.5210256248	15.6130835432
C	-13.8274065800	1.4333559923	16.0733143883
C	-14.1198185996	0.0440450052	16.6421223143
O	-13.5895738339	-0.2530045331	17.7474379992
O	-14.8406669507	-0.7232500952	15.9229090562
H	-12.5727582786	3.0632525524	14.0750691097
H	-12.1578736952	0.7074631876	14.9010854637
H	-11.7123034742	1.3339466474	16.4826414120
H	-14.0126586953	2.1831579361	16.8539012683
H	-14.5030613432	1.6309206611	15.2340791128
C	-12.1639999401	-2.3060000113	12.2389999809
C	-13.2469151861	-3.3815285490	12.0800546170
C	-13.1360796723	-4.4803538543	13.1476804812
C	-13.8078266517	-4.2350067157	14.5053800805
O	-14.6523527389	-3.2697464431	14.6088356697
O	-13.5149874219	-5.0576252833	15.4018347579
H	-12.2231220535	-1.8456133789	13.2317189326
H	-14.2389811121	-2.9179314066	12.1400824313
H	-13.1646778250	-3.8369749718	11.0821129865
H	-13.5614612882	-5.4235134720	12.7793055079
H	-12.0831652521	-4.7013194350	13.3642995012
C	-18.0649999771	-0.5230001032	12.5230001656
C	-17.2775607638	-0.6613025179	13.8238721964
C	-18.1088082590	-1.3253734056	14.9085034310
O	-19.3550335995	-1.1381757343	14.9184193389
O	-17.5122643803	-2.0601997006	15.7662410379
H	-18.3369148095	-1.5068155314	12.1208831436
H	-16.3527264554	-1.2291206054	13.6847578683
H	-16.9694266613	0.3247245054	14.1990449861
C	-21.9319999577	-3.3250000096	12.2140001622
C	-21.6630351361	-3.5685440882	13.7099148353
C	-22.4382555481	-2.5886472823	14.6114563827

C	-22.2623617294	-2.8407045578	16.1195599863
N	-20.8835356792	-2.5645475918	16.5443528776
C	-20.4287697758	-2.8128443661	17.7587028589
N	-21.2245516645	-3.2062999791	18.7742638007
N	-19.0957233345	-2.6762532008	18.0143946337
H	-21.6262650334	-2.3124645957	11.9234369786
H	-21.9367215338	-4.6010270860	13.9733592675
H	-20.5894092258	-3.4670087448	13.9070454917
H	-22.1272892539	-1.5604562833	14.3838666228
H	-23.5126219957	-2.6548580046	14.3870161522
H	-22.9620772877	-2.1986508466	16.6776560506
H	-22.5115751253	-3.8873066819	16.3504157717
H	-20.2385205765	-2.0206040640	15.8852672871
H	-22.1947331787	-3.3978217727	18.5850627967
H	-20.7856242471	-3.6993289312	19.5586398057
H	-18.4768695555	-2.3790425541	17.2331207210
H	-18.8281703321	-2.2832149704	18.9084970046
C	-16.2809998686	-5.8030000403	12.1999997685
C	-16.5841239069	-6.0490364943	13.6877296257
C	-17.3930025260	-4.8726327340	14.2898752691
C	-17.5214377307	-4.9615475208	15.7979369175
O	-18.4933051061	-5.5686810058	16.3110830822
O	-16.6078643591	-4.4367616259	16.5554506538
H	-15.7461141487	-4.8590454831	12.0606533159
H	-17.1486657976	-6.9838357260	13.8087130540
H	-15.6497616457	-6.1737666801	14.2455688181
H	-16.8883499172	-3.9406464874	14.0307728409
H	-18.4017310835	-4.8654159048	13.8599988017
C	-16.3929999515	-9.8490000276	16.0549999477
C	-16.7072950558	-8.9410522652	17.2533893888
C	-15.7673323342	-7.7402285854	17.3942812376
O	-14.6770336104	-7.7350207684	16.7760685838
O	-16.1341832173	-6.7803992701	18.1687065575
H	-16.4997657808	-9.3003296215	15.1131845843
H	-17.7363377407	-8.5609788135	17.1990198350
H	-16.6408945253	-9.5106351789	18.1932711055
C	-17.5420000293	-9.6659997195	21.8140000285
C	-17.1859147686	-8.2110353169	22.1628884304
C	-17.9150318658	-7.1325306797	21.3729292174
O	-19.1565445988	-7.2451577400	21.1464961772
O	-17.2417964895	-6.1060538902	21.0055014480
H	-18.6185334490	-9.8416195213	21.9115201071
H	-17.4253767228	-8.0255761459	23.2215894902
H	-16.1157190022	-8.0375506680	22.0452929390

C	-14.0159999799	-9.9710000234	25.1559999575
C	-14.5510401052	-8.8540454413	24.2749862447
C	-13.8996404129	-7.4902748521	24.5725700676
C	-14.4298812887	-6.4521818907	23.6052571721
O	-15.1139038255	-5.4750061389	24.0342531134
O	-14.2199096075	-6.6494586263	22.3589869959
H	-14.4937841256	-10.9319499068	24.9254071402
H	-14.3791428611	-9.0950932138	23.2200354749
H	-15.6366876317	-8.7724630300	24.4126647889
H	-14.1043914763	-7.1761103243	25.6019487008
H	-12.8142879893	-7.5606739673	24.4376494827
C	-10.0720000107	-10.4519999910	20.3670000201
C	-11.1106373369	-9.3590173252	20.6595444214
O	-11.2954401391	-8.5147427053	19.4945446432
C	-10.7536929698	-8.5211171150	21.8923549024
H	-10.3552995231	-11.0138165903	19.4708220798
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H	-10.5825432336	-7.8203427410	19.4576178015
H	-11.5277830416	-7.7761396755	22.0996126709
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H	-9.8108261816	-7.9888066365	21.7241262476
C	-9.3519999811	-7.6870000378	26.4130000280
C	-9.6569303450	-6.8578537931	25.1525532541
C	-10.1794644178	-5.4377678954	25.4642578410
C	-10.7215958453	-4.7323000913	24.2190956711
O	-11.5466054525	-5.3065070342	23.4939966518
N	-10.2789569294	-3.4822216599	23.9799630500
H	-8.5859563630	-7.2068633944	27.0360214007
H	-8.7553420952	-6.7823749743	24.5289922966
H	-10.4086427426	-7.3696044505	24.5436111677
H	-11.0162405161	-5.5123439876	26.1740633817
H	-9.3970730625	-4.8399832194	25.9517486099
H	-9.6009041866	-3.0575085928	24.5915651471
H	-10.5965045635	-2.9498312763	23.1579237847
P	-15.9216812285	-2.1854980249	19.5222964518
O	-16.4557808272	-3.5865533537	19.9186053499
O	-14.4876134532	-1.9612075977	19.9582514260
O	-16.4281154073	-1.7083512719	18.1722736043
O	-16.8741993718	-1.2349299728	20.6397061142
Ca	-13.8742551201	-5.5956043149	17.6668506391
Ca	-17.7882960491	-5.1486063404	18.6749865571
Ca	-15.4439256088	-4.6575980241	21.7735649133
Fe	-12.9371916609	-2.2257522952	18.3401445069
Fe	-15.5021100081	-2.5876534511	16.3723834200

O	-14.2838003104	-3.2448768502	17.5166801629
O	-12.3216154850	-4.2464689883	19.0960627972
O	-13.1463801880	-3.9725423828	21.7382675150
O	-16.8821902321	-2.9457379162	22.7854540874
O	-19.5667670889	-4.5645864520	20.6350587013
O	-19.7607643166	-6.6606986551	18.6085820775
O	-13.4639020243	-7.0027291674	19.6465778583
H	-7.0334283996	-7.1253623821	20.0301134651
H	-5.7843487832	-5.9128533227	20.4151957868
H	-7.5306247300	0.9753724049	21.3098732957
H	-6.8761876399	0.0714448277	22.6882717377
H	-8.5814343121	-2.2977393842	16.0025202426
H	-8.1033492105	-1.0178543879	17.1385669407
H	-12.1221358047	3.6968392643	15.6679340915
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H	-11.1615294969	-2.7418916946	12.1360561276
H	-12.2674657053	-1.5142682821	11.4855016067
H	-18.9916494719	0.0336239312	12.6889691968
H	-17.4759371137	-0.0015567345	11.7582937219
H	-21.3729892474	-4.0338014498	11.5927278745
H	-22.9983692651	-3.4370291242	11.9766788201
H	-15.6676072835	-6.6089081659	11.7785701138
H	-17.2091297538	-5.7493720365	11.6140834959
H	-15.3615893568	-10.2078088993	16.1088828885
H	-17.0680683880	-10.7132748258	16.0307486289
H	-17.2506450055	-9.9048906062	20.7841283524
H	-17.0136402583	-10.3564220864	22.4804544201
H	-12.9338001426	-10.0993018177	25.0203562270
H	-14.1904857586	-9.7619162992	26.2202754806
H	-9.0883084828	-9.9994149463	20.1918053357
H	-9.9884265381	-11.1498668627	21.2099874899
H	-10.2523390301	-7.8123475292	27.0281144571
H	-8.9871497345	-8.6849921821	26.1442170473
H	-19.6939419265	-7.2152053818	19.4152153687
H	-19.6912396891	-7.2119318680	17.8193788617
H	-18.9901920018	-4.1564065512	21.2975409482
H	-19.5834552872	-5.5282495001	20.8842829155
H	-16.9541887055	-2.1915518429	22.1590268074
H	-16.6797143597	-2.5893014007	23.6586847253
H	-12.6709141777	-3.0989778889	21.6771124408
H	-12.5585561735	-4.5249545483	22.3127176931
H	-11.2676642307	-4.3763696005	19.0993493830
H	-12.5753592025	-4.2876139811	20.0455745674
H	-12.6570912537	-7.5872976416	19.5902982965

H	-13.6880977642	-6.9845426876	20.5928876784
C	-16.7765586994	0.1257610194	20.7432004178
C	-15.6872820987	0.8685057498	20.2551917413
C	-17.8368429134	0.7728820949	21.4003232439
C	-15.6757245583	2.2471040990	20.4293500371
H	-14.8643099974	0.3729668738	19.7525325188
C	-17.8205684029	2.1487933191	21.5737026206
H	-18.6710229711	0.1784466482	21.7614556392
C	-16.7352162904	2.8774888664	21.0845583867
H	-14.8471370902	2.8420546295	20.0642715248
H	-18.6294780808	2.6679875539	22.0731262943
N	-16.7132604634	4.3249490953	21.2639428849
O	-15.7317049954	4.9467765252	20.8495565130
O	-17.6808076869	4.8536656657	21.8225514544

TS_{pnp}

Energy with the medium-sized basis set:	-5899.31850
Solution energy with the medium-sized basis set:	-5899.40777
Energy with larger basis sets:	-5901.50442
Zero-point energy:	1.66387
Imaginary frequency:	-257.8815
Dispersion effect:	-0.34744

C	-6.8650001800	-6.1059999000	20.3889998900
C	-7.7129747100	-4.9826653900	19.7878317800
C	-9.1963007800	-5.3527162300	19.5890188800
O	-9.5100240000	-6.5633176900	19.6496453100
O	-9.9572628700	-4.3565674800	19.3553075800
H	-7.2158654800	-6.3658875700	21.3948300100
H	-7.6706329600	-4.0776175300	20.4077404800
H	-7.3175353700	-4.6902281700	18.8030468700
C	-7.4140001400	-0.0290000600	21.7369999500
C	-8.7873200100	-0.6794723600	21.9840048400
C	-9.5413287400	-0.9070578400	20.6678435300
C	-10.9629347900	-1.4554981300	20.7680019500
O	-11.3647251400	-2.0195202900	21.8125695100
O	-11.6569498400	-1.2804429700	19.7060831200
H	-6.7937809700	-0.6588938400	21.0865960000
H	-8.6542277800	-1.6392829500	22.5001311300
H	-9.3879214700	-0.0452586900	22.6505460000
H	-9.5903066900	0.0275722300	20.0941879700
H	-8.9923827400	-1.6244997200	20.0407816200
C	-8.8830001000	-1.7600000100	16.9099999800

C	-10.2519231400	-1.0886197500	16.8248458700
S	-11.5843307300	-2.3367409500	16.5644120600
H	-8.8697169200	-2.4999126900	17.7168798000
H	-10.4730671200	-0.5356873200	17.7400538700
H	-10.2848268500	-0.3946431500	15.9783980000
C	-11.9689999700	2.8629999100	14.9700000900
C	-12.3751068900	1.5397165100	15.6335590400
C	-13.8460300200	1.4972418100	16.1177016700
C	-14.1539928300	0.1213648700	16.7051636700
O	-13.6152877800	-0.1755631700	17.8019789800
O	-14.8932200400	-0.6432088500	15.9942371200
H	-12.5817657200	3.0696498000	14.0827790900
H	-12.2151760200	0.7135790800	14.9273859900
H	-11.7294925300	1.3457658100	16.4965441900
H	-13.9988213700	2.2579962700	16.8940618700
H	-14.5306662200	1.7014899200	15.2876677100
C	-12.1639999300	-2.3060000000	12.2389999700
C	-13.2616213900	-3.3813668000	12.2166900000
C	-13.1136250000	-4.4184834900	13.3448826700
C	-13.7963612900	-4.1304409500	14.6876422500
O	-14.6350803700	-3.1541973900	14.7502114300
O	-13.5204245600	-4.9123857900	15.6224891500
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H	-14.2450741100	-2.9030170100	12.2966280500
H	-13.2357718300	-3.9000367200	11.2472143500
H	-13.5093791100	-5.3924536200	13.0255520500
H	-12.0549755800	-4.5963637300	13.5729751700
C	-18.0649999400	-0.5230001500	12.5230002600
C	-17.3473835800	-0.5031081000	13.8753958100
C	-18.1617688100	-1.2363890800	14.9294699500
O	-19.4057983200	-1.0627297500	14.9602954600
O	-17.5569870300	-2.0276611600	15.7362613200
H	-18.1707220700	-1.5493337900	12.1502325500
H	-16.3500199600	-0.9451228600	13.8123439700
H	-17.2103376000	0.5323838400	14.2177169900
C	-21.9319999500	-3.3250000100	12.2140001700
C	-21.6527058300	-3.5669839000	13.7104080800
C	-22.4512335900	-2.6133762200	14.6213646400
C	-22.2835584000	-2.8772447300	16.1299300400
N	-20.9179040500	-2.5689314900	16.5767850700
C	-20.4694768600	-2.8099821300	17.7972040500
N	-21.2636952800	-3.2217429000	18.8033651300
N	-19.1400840900	-2.6545379000	18.0612317200
H	-21.6579800000	-2.3024798200	11.9265658300

H	-21.8977537200	-4.6077669300	13.9689026400
H	-20.5814364700	-3.4391960600	13.9058564700
H	-22.1607665100	-1.5762248900	14.4076204800
H	-23.5227841300	-2.6986262300	14.3899523000
H	-23.0069231700	-2.2595308700	16.6851031200
H	-22.5066277500	-3.9322523900	16.3477961900
H	-20.2846673200	-2.0116292300	15.9303461800
H	-22.2314281900	-3.4239732700	18.6137628900
H	-20.8192926100	-3.6851333700	19.6044427000
H	-18.5283879200	-2.3507989600	17.2856673000
H	-18.8608519200	-2.2600493000	18.9548844800
C	-16.2809998500	-5.8030000400	12.1999997500
C	-16.5774881900	-6.0165505000	13.6953203500
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C	-17.5216082500	-4.9037033900	15.7937071700
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H	-15.7174304200	-4.8784484300	12.0394115100
H	-17.1566800200	-6.9394080100	13.8361972900
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C	-15.8564321000	-7.7256040000	17.4116048400
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O	-16.2743473000	-6.7924318300	18.1906334800
H	-16.4927667200	-9.3052566200	15.1093518100
H	-17.7948735300	-8.5946227800	17.1611480200
H	-16.7046201200	-9.5175432400	18.1842876200
C	-17.5420000200	-9.6659996800	21.8140000100
C	-17.3344898800	-8.2066370200	22.2577817800
C	-18.0212774800	-7.1650102600	21.3843259500
O	-19.2618179700	-7.2773911400	21.1419163500
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C	-14.0159999600	-9.9709999800	25.1559999500
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C	-14.5949095400	-6.4413711200	23.6832232500
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C	-11.1485100600	-9.4045585500	20.7057620700
O	-11.3490820500	-8.4975633400	19.5914131600
C	-10.8316116100	-8.6281113200	21.9900921500
H	-10.3291286200	-10.9711521000	19.4379063400
H	-12.1126739300	-9.9193151900	20.8201269300
H	-10.6489943200	-7.7914724900	19.6007980700
H	-11.6294815700	-7.9149499200	22.2222118900
H	-10.7154399100	-9.3134031800	22.8401309900
H	-9.9016460400	-8.0620157200	21.8653283300
C	-9.3519999800	-7.6870000500	26.4130000300
C	-9.7412036700	-6.8579250700	25.1748674400
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C	-10.8130574200	-4.7044627300	24.3084461600
O	-11.7172028800	-5.2265171400	23.6400966900
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H	-9.5661941100	-3.1045164200	24.5987615600
H	-10.6331973200	-2.9422408000	23.2231075700
P	-15.8032878900	-2.3570443200	19.3294918100
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O	-14.5713177400	-1.8183806000	20.0341793800
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Ca	-14.1005862400	-5.4830385600	17.8473284300
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Fe	-15.6051157500	-2.4766615400	16.4113081400
O	-14.5122226500	-3.0810762100	17.8048431900
O	-12.4346259300	-4.1566128100	19.2251912900
O	-13.3176144200	-3.8836058700	21.8809317700
O	-17.6036372700	-3.3295675500	22.4057381400
O	-19.5804751300	-4.5155675000	20.6780228400
O	-19.8792857900	-6.6552588100	18.6435154500

O	-13.5408366400	-6.9556247800	19.7456895400
H	-6.9425943900	-7.0101504800	19.7779336900
H	-5.8083258900	-5.8163827800	20.4597630700
H	-7.5246295500	0.9465530300	21.2465175500
H	-6.8660816500	0.1274959500	22.6747715200
H	-8.6394297600	-2.2803082800	15.9758749900
H	-8.0985036800	-1.0129059500	17.0992065000
H	-12.0891307900	3.7075935200	15.6612646500
H	-10.9192095300	2.8357013500	14.6532178000
H	-11.1706851700	-2.7570913300	12.1167639600
H	-12.3046818200	-1.5726509800	11.4347527500
H	-19.0671291800	-0.0947227700	12.6144911700
H	-17.5069343700	0.0485990700	11.7715878700
H	-21.3528479800	-4.0146140700	11.5896266800
H	-22.9949694200	-3.4684253500	11.9786550200
H	-15.6954767900	-6.6341815700	11.7880770100
H	-17.2120021500	-5.7305610000	11.6213264700
H	-15.3535163100	-10.1799171600	16.1323791800
H	-17.0427857900	-10.7318688400	16.0158625800
H	-17.1135108900	-9.8360908800	20.8191658800
H	-17.0495877900	-10.3505361700	22.5132268900
H	-12.9263364100	-10.0212602300	25.0297981700
H	-14.2157278300	-9.8123120800	26.2245329300
H	-9.1001521400	-9.9623097100	20.2302819900
H	-9.9795102800	-11.1916958000	21.1723939300
H	-10.2071815100	-7.8079248600	27.0902929000
H	-9.0105329800	-8.6866677900	26.1208735300
H	-19.7874918200	-7.1389365700	19.5009997900
H	-19.8341309900	-7.2864797600	17.9155082000
H	-19.0115442300	-4.1183573800	21.3704987600
H	-19.6521476900	-5.4681629200	20.9310231900
H	-17.4800085900	-2.5557905300	21.7540872600
H	-17.7873477500	-2.9632181000	23.2793704000
H	-12.8535520900	-3.0120261000	21.8110983500
H	-12.7259046700	-4.4250683900	22.4637977500
H	-11.3842123700	-4.3235132300	19.2298971600
H	-12.6910474500	-4.1951256300	20.1737496800
H	-12.7407905200	-7.5433191300	19.6727776500
H	-13.7665593000	-6.9652176000	20.6922934500
C	-17.2811788100	-0.2984309400	20.8740873400
C	-16.3230607100	0.6813757600	20.5306042700
C	-18.4570347900	0.1025430700	21.5495446100
C	-16.5471093600	2.0107158300	20.8554191600
H	-15.4099554400	0.3803638500	20.0314751200

C	-18.6765583700	1.4310829300	21.8760728200
H	-19.1980109200	-0.6516293700	21.8027233100
C	-17.7173765800	2.3838898900	21.5251291300
H	-15.8188555800	2.7723914400	20.6029556800
H	-19.5758585000	1.7477713400	22.3907330400
N	-17.9410874000	3.7783663200	21.8658381900
O	-17.0767388300	4.6027887300	21.5490803400
O	-18.9871320600	4.0736822500	22.4582588900

Int_{pnp}

Energy with the medium-sized basis set:	-5899.36634
Solution energy with the medium-sized basis set:	-5899.45371
Energy with larger basis sets:	-5901.55446
Zero-point energy:	1.66500
Dispersion effect:	-0.34152

C	-6.8650001749	-6.1059999092	20.3889999102
C	-7.6784426553	-5.0115209212	19.6878161449
C	-9.1591012721	-5.3742514657	19.4576957706
O	-9.4988772194	-6.5688636454	19.5895411153
O	-9.8978442011	-4.3836620381	19.1249244155
H	-7.2534172259	-6.2967831369	21.3961643201
H	-7.6450623163	-4.0698561554	20.2512572635
H	-7.2440276501	-4.7853727627	18.7019056238
C	-7.4140001629	-0.0290000613	21.7369999107
C	-8.7545207058	-0.7571189298	21.9056838451
C	-9.5990651101	-0.6389354285	20.6357537516
C	-10.9345417409	-1.3700833376	20.6375941128
O	-11.3213075756	-2.0181514097	21.6295499272
O	-11.5894229844	-1.2177866715	19.5389032290
H	-6.8399421807	-0.4539000128	20.9038429314
H	-8.5789202585	-1.8175895033	22.1290162997
H	-9.3080349194	-0.3424978376	22.7591611442
H	-9.8068228063	0.4173076088	20.4097800992
H	-9.0360179040	-1.0225586215	19.7743890309
C	-8.8830001188	-1.7600000327	16.9100000145
C	-10.2301387408	-1.1056647947	16.6141067045
S	-11.5353091329	-2.3897822949	16.3914721134
H	-8.9535565840	-2.4183804932	17.7817106358
H	-10.5275072374	-0.4459089469	17.4314161148
H	-10.1849935904	-0.5216076900	15.6886847073
C	-11.9689999692	2.8629998642	14.9700001473

C	-12.3877412918	1.5133298903	15.5710912127
C	-13.8740555350	1.4393986185	16.0002149563
C	-14.1859400199	0.0638636082	16.5889057690
O	-13.5683656331	-0.2700353327	17.6276580812
O	-15.0281680034	-0.6575003430	15.9447232973
H	-12.5504603819	3.0990131214	14.0692587480
H	-12.1916156369	0.7140453305	14.8429690087
H	-11.7724380205	1.2959327528	16.4498870318
H	-14.0696723812	2.1973747066	16.7707553515
H	-14.5358741962	1.6341914002	15.1500291484
C	-12.1639999249	-2.3060000082	12.2389999982
C	-13.2766587109	-3.3655288718	12.1893493668
C	-13.1613492727	-4.4156967920	13.3099631700
C	-13.8768475959	-4.1452075559	14.6380290797
O	-14.7397073522	-3.1815319753	14.6770408397
O	-13.6111274025	-4.9170098503	15.5793949553
H	-12.1751708130	-1.7783837300	13.1998025811
H	-14.2552529698	-2.8753041518	12.2549100078
H	-13.2410325201	-3.8761869318	11.2163911381
H	-13.5527949914	-5.3840864133	12.9696816989
H	-12.1099119784	-4.6003851424	13.5634480489
C	-18.0649998943	-0.5230001898	12.5230003462
C	-17.5451501105	-0.0949467724	13.9100765278
C	-18.2546707441	-0.9263783042	14.9648690669
O	-19.4500575340	-0.6831687771	15.2163525737
O	-17.6236858940	-1.9255255577	15.4954065651
H	-17.8317483143	-1.5759766991	12.3248444461
H	-16.4639774113	-0.2264459656	13.9857800843
H	-17.7819492953	0.9616327533	14.0820436546
C	-21.9319999468	-3.3250000064	12.2140001702
C	-21.6890609988	-3.4853324643	13.7259293089
C	-22.4196341472	-2.4134195579	14.5576944454
C	-22.3579020666	-2.6439921819	16.0775411276
N	-21.0032212028	-2.4410086764	16.6081916373
C	-20.6245394502	-2.8483373619	17.8155763096
N	-21.4778879275	-3.4293659528	18.6717678287
N	-19.3324841770	-2.7006244748	18.2165607852
H	-21.5866548949	-2.3449287702	11.8613227811
H	-22.0235552474	-4.4830300517	14.0468468045
H	-20.6132994730	-3.4389940657	13.9363717072
H	-22.0114580490	-1.4206289403	14.3260620720
H	-23.4816517302	-2.3943203809	14.2732215027
H	-23.0621306994	-1.9627967624	16.5795907913
H	-22.6758054341	-3.6736685239	16.2953862357

H	-20.3605730803	-1.8003132938	16.0873604227
H	-22.4428536978	-3.5474455146	18.4156876092
H	-21.0790485014	-3.9945431228	19.4372555898
H	-18.6578371296	-2.2864159236	17.5767209963
H	-19.1499814152	-2.4969124557	19.2129180248
C	-16.2809998295	-5.8030000433	12.1999997419
C	-16.6378038231	-6.0220591292	13.6802660369
C	-17.5579876256	-4.8953126638	14.2196138977
C	-17.6650024164	-4.9231884249	15.7344064334
O	-18.5996095394	-5.5331696149	16.2965393197
O	-16.7379475201	-4.3465746661	16.4412295724
H	-15.7843769710	-4.8380078357	12.0558125655
H	-17.1387021366	-6.9911548419	13.8074837112
H	-15.7236832586	-6.0675276675	14.2820291190
H	-17.1518399779	-3.9291522936	13.9087754825
H	-18.5626859203	-5.0044217030	13.7959863817
C	-16.3929999525	-9.8490000256	16.0549999349
C	-16.8109740147	-8.9179710328	17.1858696629
C	-15.8732039118	-7.7304254610	17.3611812423
O	-14.7721369879	-7.6985530463	16.7614087636
O	-16.2610922950	-6.7907313603	18.1433704836
H	-16.3944030553	-9.3215345553	15.0953511996
H	-17.8196258020	-8.5187515861	17.0130887456
H	-16.8466067415	-9.4534941281	18.1463676779
C	-17.5420000301	-9.6659996739	21.8140000145
C	-17.2341070221	-8.2162596080	22.2405930505
C	-18.0090756118	-7.1313532923	21.5000689923
O	-19.2530221133	-7.2816332709	21.3178243344
O	-17.3691060297	-6.0909294558	21.1098463988
H	-18.6108599474	-9.8831554773	21.9102581303
H	-17.4798608753	-8.0976062661	23.3067364202
H	-16.1712435763	-8.0028451781	22.1271086910
C	-14.0159999668	-9.9709999740	25.1559999444
C	-14.5632075094	-8.8640571199	24.2640934735
C	-13.9083327655	-7.4932624852	24.5256821065
C	-14.4590164290	-6.4533597172	23.5660748348
O	-15.1217434978	-5.4720135474	24.0109469810
O	-14.2789806285	-6.6451028149	22.3127584744
H	-14.5021510046	-10.9326600192	24.9475384352
H	-14.4118972291	-9.1246607531	23.2102823376
H	-15.6454758752	-8.7796598659	24.4204491328
H	-14.0886656786	-7.1682121719	25.5562693551
H	-12.8260299730	-7.5646097781	24.3663932662
C	-10.0720000074	-10.4520000220	20.3670000206

C	-11.1577618872	-9.4035297220	20.6472384627
O	-11.3172375954	-8.5267349462	19.5008762024
C	-10.8822653197	-8.5959167911	21.9202559347
H	-10.2959933793	-10.9921062181	19.4412180047
H	-12.1261878210	-9.9141048740	20.7401315751
H	-10.6181245009	-7.8227566167	19.5189446655
H	-11.6832313834	-7.8755135807	22.1099635200
H	-10.7984814330	-9.2620636249	22.7890167392
H	-9.9463436611	-8.0360234850	21.8152782533
C	-9.3520000117	-7.6869999377	26.4129998865
C	-9.6488494450	-6.8675027216	25.1426556607
C	-10.2534125311	-5.4759075677	25.4388239800
C	-10.7518188029	-4.7723913408	24.1749064050
O	-11.5194825094	-5.3546380142	23.3976033761
N	-10.3260559858	-3.5071986837	23.9713841425
H	-8.6365137575	-7.1712392171	27.0667535281
H	-8.7271991734	-6.7434468199	24.5570880943
H	-10.3486200051	-7.4137147568	24.5022367846
H	-11.1264671664	-5.5977678781	26.0959215488
H	-9.5282713300	-4.8527918254	25.9800605383
H	-9.7137144430	-3.0600785994	24.6339555958
H	-10.6274881638	-2.9722457971	23.1519017334
P	-15.4827792519	-2.7653471007	18.8865314059
O	-15.9509126812	-4.1369666038	19.4582000864
O	-14.5934839923	-1.9978909218	19.8628696209
O	-16.6034967863	-2.0210317021	18.1216254270
O	-18.9306098881	-2.3769986521	21.0697881205
Ca	-14.1020804165	-5.5697085064	17.8256016305
Ca	-17.9748493777	-5.2720945607	18.7042165227
Ca	-15.5261485289	-4.6217521910	21.7668688109
Fe	-12.8098242635	-2.1275991087	18.3525839152
Fe	-15.8490346168	-2.4652158079	16.1793415818
O	-14.4957897925	-3.1269269057	17.6377895921
O	-12.3572620737	-4.1531968312	19.0389390352
O	-13.1519780672	-4.0074075554	21.6622319298
O	-16.4359226132	-2.3981599297	22.0468999484
O	-19.8054307541	-4.7168573616	20.3998353820
O	-19.6972779204	-7.0695507581	18.7075415369
O	-13.4753617033	-6.9867522164	19.6764659172
H	-6.9325523374	-7.0460966028	19.8335899680
H	-5.8084443584	-5.8219755712	20.4768535417
H	-7.5674782001	1.0370017316	21.5244247395
H	-6.7950507799	-0.1029476424	22.6398392198
H	-8.5464951425	-2.3709490839	16.0638923788

H	-8.1192452725	-0.9918397028	17.0987103959
H	-12.1201461456	3.6804101487	15.6871550176
H	-10.9084601371	2.8536186063	14.6909383111
H	-11.1756928877	-2.7701832270	12.1276380360
H	-12.2821936350	-1.5641026656	11.4392409630
H	-19.1510416359	-0.3939640684	12.4657270035
H	-17.6039732460	0.0768369624	11.7296258910
H	-21.3967494919	-4.0928320301	11.6436774501
H	-22.9999099570	-3.4100143877	11.9732427877
H	-15.6118576861	-6.5902548135	11.8318883843
H	-17.1820588372	-5.8111606087	11.5715724212
H	-15.3772215121	-10.2202288667	16.2175309169
H	-17.0706814858	-10.7083937400	15.9753466613
H	-17.2499954266	-9.8374669526	20.7706481814
H	-16.9837559120	-10.3720963665	22.4383112205
H	-12.9365068798	-10.1059516639	25.0053154457
H	-14.1734346805	-9.7434992244	26.2190162509
H	-9.0967238451	-9.9631701838	20.2526839295
H	-10.0033853025	-11.1751158908	21.1896546858
H	-10.2682778856	-7.8607690122	26.9913510454
H	-8.9267438589	-8.6636998736	26.1553340456
H	-19.6877810465	-7.3722406909	19.6475057010
H	-19.5708688658	-7.8413864157	18.1448391099
H	-19.4898651108	-3.9213181634	20.9215639400
H	-19.7590352775	-5.5390176591	20.9394560781
H	-17.3563528888	-2.2811341067	21.6866019222
H	-15.8541832266	-1.8364363836	21.5019745131
H	-12.7066628480	-3.1257337081	21.6412838720
H	-12.5629612419	-4.5698772886	22.2254268464
H	-11.2912987905	-4.3455307812	19.0286667507
H	-12.6020961112	-4.2213649013	19.9947454575
H	-12.6818881287	-7.5838408135	19.6051353059
H	-13.7175535305	-6.9871055657	20.6208793425
C	-19.6900241895	-1.4066103371	21.5360101505
C	-19.3821993550	-0.0461000881	21.2559558785
C	-20.8420085988	-1.6695986262	22.3282128117
C	-20.1692609297	0.9819061723	21.7389244643
H	-18.5078170697	0.1675877535	20.6474200395
C	-21.6314512073	-0.6413443422	22.8115402700
H	-21.0868052045	-2.7036207863	22.5554024588
C	-21.2963424792	0.6865083395	22.5180252494
H	-19.9348029295	2.0186831559	21.5276352864
H	-22.5068722735	-0.8377823788	23.4197265627
N	-22.1173497616	1.7634030843	23.0196741261

O	-21.7877944846	2.9266204062	22.7501708933
O	-23.1152983813	1.4799666671	23.6980397732

React_{base}

Energy with the medium-sized basis set:	-5579.51807
Solution energy with the medium-sized basis set:	-5579.59182
Energy with larger basis sets:	-5581.60487
Zero-point energy:	1.63387
Dispersion effect:	-0.34823

C	-6.48640900	3.65381000	2.99202500
C	-5.07725900	4.02725500	2.52339100
C	-4.16097300	2.81120200	2.31091800
O	-4.45850500	1.73951700	2.87478900
O	-3.14507500	3.04345400	1.56477400
H	-7.00404300	3.05195100	2.23559900
H	-5.10396900	4.60483800	1.59134100
H	-4.58772300	4.67549800	3.26633600
C	-5.44101400	6.42022100	-2.51275000
C	-4.95682600	4.95257700	-2.57960300
C	-3.52475100	4.76922500	-2.04471400
C	-2.95415700	3.34282400	-2.07004400
O	-3.70107900	2.38191400	-2.40102800
O	-1.72568900	3.21761000	-1.76008500
H	-5.43163300	6.78896700	-1.47943800
H	-5.64034300	4.31759200	-2.00082300
H	-5.00556300	4.59516200	-3.61778300
H	-2.82840900	5.41315000	-2.59990100
H	-3.47162900	5.09895200	-0.99761800
C	-1.44630200	6.04134600	1.00193100
C	-0.53483600	5.79635700	-0.20801900
S	0.65250200	4.42107600	0.10771500
H	-2.05041300	5.15552700	1.22279200
H	-1.11609100	5.55411600	-1.09813300
H	0.06933900	6.68671500	-0.42427700
C	3.17033500	7.28188700	-2.43417700
C	3.31727100	5.75204700	-2.39290300
C	4.14920200	5.25493000	-1.18597400
C	4.14420400	3.72974300	-1.10996100
O	4.52349200	3.07763600	-2.11536300
O	3.71526500	3.21151100	-0.01663600
H	2.66805400	7.65167600	-1.53118300

H	2.32060200	5.29564900	-2.33787200
H	3.78320900	5.38651000	-3.31598400
H	5.18887300	5.59962200	-1.28993500
H	3.74556700	5.65643900	-0.25221100
C	3.86160200	5.01558600	2.91381100
C	3.40460100	4.20600400	4.14284000
C	1.99530200	3.59159300	4.01495100
C	1.86404500	2.36458000	3.11184400
O	2.87687700	2.09219600	2.36089200
O	0.81129600	1.69366600	3.16493100
H	3.87342000	4.39055600	2.01881000
H	4.12756000	3.40278200	4.33759100
H	3.41303800	4.85712800	5.03044600
H	1.60524400	3.30147900	4.99940600
H	1.29115800	4.33910200	3.61948500
C	7.71808700	1.74526500	-0.62371100
C	6.91668700	1.38377100	0.62830300
C	5.93873500	0.27360000	0.28030800
O	6.39153800	-0.74023500	-0.30596200
O	4.71914100	0.42743000	0.60203100
H	8.23024000	0.86216700	-1.01623900
H	7.58889400	1.02084100	1.41931300
H	6.36616900	2.24463600	1.01753700
C	9.49156700	-2.59961600	0.31285000
C	8.18901100	-3.32409100	-0.07020100
C	7.95795600	-3.32736400	-1.59509600
C	6.56565200	-3.81809900	-2.03851000
N	5.55091200	-2.77078100	-1.84140600
C	4.39051900	-2.74466800	-2.47191900
N	4.02936400	-3.71294300	-3.35233700
N	3.51436400	-1.73279000	-2.24211100
H	9.42908700	-1.54202300	0.03285700
H	8.21038000	-4.36222200	0.29448200
H	7.35221100	-2.82170000	0.42543500
H	8.10317400	-2.31268700	-1.98738600
H	8.71386700	-3.96565000	-2.07492400
H	6.59554700	-4.07430100	-3.10584700
H	6.29027800	-4.72780000	-1.48305700
H	5.76790500	-1.98322300	-1.18043900
H	4.44419200	-4.61976400	-3.19331200
H	3.02232700	-3.76437200	-3.52946500
H	3.84856600	-0.89393000	-1.76258000
H	2.86143300	-1.45601400	-2.98914500
C	5.38835800	-0.02075200	4.13222500

C	4.03866100	-0.60719900	3.69517100
C	4.21474100	-1.71640500	2.64856700
C	3.27383700	-1.75581300	1.45199000
O	3.36272400	-2.79135900	0.73833400
O	2.43351600	-0.81751600	1.17170100
H	5.89032700	0.44923900	3.27978600
H	3.49149100	-0.99449800	4.56480900
H	3.43174300	0.19320900	3.27501100
H	5.21618500	-1.65842500	2.20044600
H	4.16389900	-2.71355100	3.10615700
C	1.43932500	-3.89148700	4.94845600
C	0.94179900	-4.07751300	3.50316300
C	0.54129400	-2.76926300	2.81224700
O	0.37858300	-1.74212700	3.51705800
O	0.39190600	-2.77466200	1.53572600
H	2.33835900	-3.26700900	4.97415600
H	1.70189500	-4.56985200	2.88295600
H	0.06457900	-4.74175300	3.48130400
C	-2.10643300	-6.65002800	1.16192400
C	-2.13688900	-5.57321500	0.06818900
C	-0.77043200	-5.08178500	-0.39934800
O	0.23642300	-5.78697700	-0.17487500
O	-0.73837500	-3.94914700	-1.02794900
H	-1.53857900	-7.52625600	0.83411200
H	-2.66026900	-5.95580900	-0.82279800
H	-2.70584900	-4.69911400	0.39395000
C	-6.81259900	-5.48643600	0.72292600
C	-5.56566100	-4.90962500	0.08409300
C	-5.86389700	-3.74132300	-0.87352200
C	-4.56145700	-3.06711600	-1.24152900
O	-4.21925900	-2.94243200	-2.46262100
O	-3.81841900	-2.69371000	-0.27842600
H	-6.57178900	-6.31541600	1.40033600
H	-4.89397700	-4.54105600	0.86451400
H	-5.02412500	-5.69602500	-0.45840600
H	-6.38743700	-4.08065600	-1.77383800
H	-6.49248300	-2.99916400	-0.36414400
C	-5.76198400	-1.24350600	5.15178300
C	-5.01919200	-1.51980200	3.83562800
O	-3.82929900	-0.69329400	3.74479000
C	-5.91344000	-1.33082000	2.60461200
H	-5.08578400	-1.37202600	6.00321100
H	-4.63726800	-2.54964100	3.85633400
H	-4.08226400	0.22805700	3.47919000

H	-5.37263700	-1.57217800	1.68507300
H	-6.80019400	-1.97588100	2.66871400
H	-6.24202900	-0.28798800	2.53508200
C	-9.92032600	-1.21575800	-0.08512100
C	-8.63881800	-0.37371000	-0.10548400
C	-8.08032400	-0.16996500	-1.52898600
C	-6.65672400	0.37785500	-1.49814100
O	-5.81262300	-0.15806100	-0.76798700
N	-6.38911100	1.43387700	-2.29317400
H	-10.72009500	-0.74999200	-0.67620200
H	-8.82480500	0.60647300	0.35538800
H	-7.86304400	-0.85585300	0.49777000
H	-8.03606300	-1.14247200	-2.04072400
H	-8.74810100	0.47314400	-2.11845500
H	-7.11673200	1.83655300	-2.86115600
H	-5.45074600	1.85167000	-2.32824700
P	0.28866200	-0.13163000	-2.73923200
O	0.06654000	-1.01483500	-1.47488800
O	0.49717500	1.36156700	-2.45656100
O	1.28284300	-0.76349200	-3.71245900
O	-1.22474200	-0.29465900	-3.43682900
Ca	0.04519200	-0.11083000	1.75558900
Ca	1.43162000	-2.83644200	-0.65359600
Ca	-2.06071000	-2.00345800	-1.70216000
Fe	-0.15901300	2.37528600	-0.67012700
Fe	2.95526500	1.38350800	0.50262200
O	1.16213700	1.45247500	0.19868100
O	-1.56937400	1.44770900	0.59680400
O	-3.16306300	0.09376700	-1.19207500
O	-1.92462400	-3.18204900	-3.95858300
O	1.17925300	-3.35007300	-3.24729600
O	2.67622700	-5.01504100	-0.79802600
O	-2.22603600	-1.20576400	1.67164700
H	-6.43539400	3.05274400	3.90451800
H	-7.09152100	4.54774300	3.19031300
H	-4.79320200	7.07744700	-3.10689900
H	-6.46382200	6.51728200	-2.89674800
H	-0.85295100	6.27719100	1.89316100
H	-2.12000900	6.89005800	0.80882900
H	4.14903500	7.77701400	-2.49705800
H	2.57793000	7.59848000	-3.30163600
H	3.18031100	5.85762100	2.72987300
H	4.86810400	5.42699300	3.07220200
H	7.05339700	2.13370400	-1.40388800

H	8.46929200	2.51610700	-0.40868100
H	9.67123100	-2.65154700	1.39303000
H	10.36183900	-3.03823000	-0.19468500
H	5.25950100	0.74645900	4.90619600
H	6.05696700	-0.79400700	4.53790500
H	0.67880100	-3.39191100	5.55461300
H	1.67799500	-4.86002700	5.40541800
H	-1.62568400	-6.26721500	2.06886200
H	-3.12387500	-6.96625800	1.42086900
H	-7.34243300	-4.72436400	1.30962500
H	-7.51705900	-5.86970800	-0.02826900
H	-6.13758600	-0.21292900	5.16302100
H	-6.61410100	-1.92466800	5.27127000
H	-9.73913800	-2.21544700	-0.50051400
H	-10.29272400	-1.34176800	0.93814300
H	1.83792700	-5.49807600	-0.56164700
H	3.16628400	-4.87142000	0.02595700
H	1.09583300	-2.42532500	-3.61736600
H	0.32349100	-3.79021100	-3.36071300
H	-1.88947600	-2.47440500	-4.61650400
H	-2.87033600	-3.39336500	-3.82955400
H	-3.22455300	0.90024300	-1.77256700
H	-4.09044300	-0.01981600	-0.86730800
H	-2.26418300	2.13457800	1.12626300
H	-2.18900000	0.89897100	0.05411900
H	-2.82255300	-1.00245900	2.44428200
H	-2.68643600	-1.92569600	1.21674200
C	-1.60941400	0.65260100	-4.45176500
H	-2.64700700	0.43576300	-4.71511600
H	-1.53750300	1.66790600	-4.06016700
H	-0.96613200	0.54056800	-5.33217500
O	3.20218500	0.96982500	-1.64395600
H	3.84325300	1.71014500	-1.92915800
H	2.33424900	1.22007200	-2.02648300

TS_{base}

Energy with the medium-sized basis set:	-5579.46004
Solution energy with the medium-sized basis set:	-5579.53941
Energy with larger basis sets:	-5581.54342
Zero-point energy:	1.63253
Imaginary frequency:	-176.0818
Dispersion effect:	-0.34889

C	-6.9441129999999998	3.1752560000000001	2.9292670000000003
C	-5.7204689999999996	3.5225800000000000	2.0713979999999999
C	-4.5984900000000000	2.4634079999999998	2.0749000000000000
O	-4.7771610000000004	1.4063829999999999	2.7095210000000001
O	-3.5625650000000002	2.8080639999999999	1.4014430000000000
H	-7.3995629999999997	2.2382019999999998	2.5931690000000001
H	-6.0179879999999999	3.6738430000000002	1.0234820000000000
H	-5.2764870000000004	4.4752159999999996	2.3927550000000002
C	-5.8335689999999998	6.1992950000000002	-2.4251990000000001
C	-5.2838700000000003	4.7741639999999999	-2.6092559999999998
C	-3.9315199999999999	4.6241279999999998	-1.9065140000000000
C	-3.2002429999999999	3.2954050000000001	-2.0582479999999999
O	-3.7899690000000001	2.2669049999999999	-2.4512309999999999
O	-1.9630019999999999	3.3502320000000001	-1.7261380000000000
H	-5.9178889999999997	6.4507669999999999	-1.3604300000000000
H	-5.9953450000000004	4.0422060000000002	-2.2058740000000001
H	-5.1741320000000002	4.5483960000000003	-3.6787839999999998
H	-3.2487849999999998	5.4164870000000001	-2.2395309999999999
H	-4.0576689999999997	4.7644490000000008	-0.8225789999999999
C	-2.0124330000000001	6.0146269999999999	1.2922020000000001
C	-1.0271889999999999	5.7250259999999997	0.1507240000000000
S	0.0309620000000000	4.2654350000000001	0.5223270000000000
H	-2.6855330000000004	5.1642580000000011	1.4425460000000001
H	-1.5568139999999999	5.5196889999999996	-0.7800740000000000
H	-0.3599700000000000	6.5815599999999996	-0.0045900000000000
C	2.6654790000000004	7.7270029999999998	-1.8453180000000000
C	2.3228890000000000	6.2602989999999998	-1.5339449999999999
C	3.4953050000000001	5.2920220000000002	-1.8174859999999999
C	3.1481360000000000	3.8408989999999998	-1.4889190000000001
O	2.9117169999999999	3.0506210000000000	-2.4273560000000001
O	3.1556660000000001	3.5395580000000000	-0.2342040000000000
H	3.4257990000000000	8.1122379999999996	-1.1534040000000003
H	2.0358109999999998	6.1584170000000000	-0.4815520000000000
H	1.4528559999999999	5.9488779999999997	-2.1266690000000001
H	3.7757540000000001	5.3438949999999998	-2.8752170000000006
H	4.3601869999999998	5.5908040000000003	-1.2098679999999999
C	3.2520410000000002	5.3420490000000003	3.4634380000000000
C	3.0682510000000001	4.2879050000000003	4.5687129999999998
C	1.7816069999999999	3.4540980000000001	4.4322450000000000
C	1.7399519999999999	2.4501949999999999	3.2862060000000000
O	2.7698399999999999	2.4511609999999999	2.4861650000000002
O	0.7643700000000000	1.6942699999999999	3.1725850000000002
H	3.2274870000000000	4.8810650000000004	2.4727120000000000

H	3.9338069999999998	3.6135250000000001	4.5792489999999999
H	3.0488890000000000	4.7877419999999997	5.5480630000000000
H	1.5843190000000000	2.8863219999999998	5.3512789999999999
H	0.9104900000000000	4.1110480000000003	4.2950140000000001
C	7.5382899999999999	2.5040209999999998	0.0494650000000000
C	6.0819970000000003	2.6385939999999999	-0.3722970000000000
C	5.5207980000000010	1.2613580000000000	-0.6656970000000000
O	6.2586870000000001	0.4440730000000000	-1.2560579999999999
O	4.3322269999999996	0.9599560000000000	-0.2813620000000000
H	7.6287520000000013	1.9165350000000001	0.9717330000000000
H	5.4791530000000002	3.1473599999999999	0.3818940000000000
H	6.0069629999999998	3.2358720000000001	-1.2919170000000000
C	9.6006389999999993	-1.7184280000000001	0.9539020000000000
C	8.2394700000000007	-2.1397510000000000	0.3572830000000000
C	8.3367540000000009	-2.5602109999999998	-1.1255320000000000
C	7.0513290000000000	-3.1691050000000001	-1.7246930000000000
N	5.9773639999999997	-2.1737440000000001	-1.8185629999999999
C	4.8217720000000002	-2.3364010000000000	-2.4503070000000000
N	4.5439340000000001	-3.3935300000000002	-3.2333449999999999
N	3.8523220000000000	-1.3990050000000001	-2.2753200000000002
H	10.0366350000000004	-0.8862770000000000	0.3874510000000000
H	7.8261830000000012	-2.9742299999999999	0.9423710000000000
H	7.5320669999999996	-1.3074650000000001	0.4543610000000001
H	8.6354410000000001	-1.6954970000000000	-1.7337419999999999
H	9.1312160000000002	-3.3125110000000002	-1.2335560000000001
H	7.2811170000000001	-3.5589330000000006	-2.7272870000000000
H	6.7194210000000005	-4.0151060000000003	-1.1052180000000000
H	6.1297800000000002	-1.2100709999999999	-1.4547939999999999
H	5.1431690000000003	-4.2014209999999999	-3.1839520000000001
H	3.5459079999999998	-3.5563099999999999	-3.4251140000000002
H	4.0872299999999999	-0.5874549999999999	-1.7024530000000000
H	3.2247550000000000	-1.1653640000000001	-3.0488450000000000
C	5.1090530000000003	0.4018700000000000	4.6151140000000010
C	4.1130979999999999	-0.4419900000000000	3.8155440000000000
C	4.6286600000000000	-0.6648560000000000	2.3794680000000001
C	3.5566530000000003	-1.0896200000000000	1.3958969999999999
O	3.6676560000000000	-2.1775479999999998	0.7910410000000000
O	2.5503749999999998	-0.2933740000000000	1.2104950000000001
H	5.2260819999999999	1.3913700000000000	4.1562310000000000
H	3.9456739999999999	-1.4098940000000000	4.3056680000000007
H	3.1425809999999998	0.0598950000000000	3.7795999999999998
H	5.0413800000000002	0.2829470000000000	2.0133450000000002
H	5.4366779999999997	-1.4038600000000001	2.3675760000000001
C	1.4436530000000001	-3.7905259999999998	5.0971330000000004

C	1.3164450000000001	-3.8735110000000001	3.5598999999999998
C	0.8585420000000000	-2.5837089999999998	2.8646080000000000
O	0.5597870000000000	-1.5825389999999999	3.5615650000000003
O	0.7996770000000000	-2.5746699999999998	1.5805530000000003
H	2.1811120000000002	-3.0349879999999998	5.3874160000000000
H	2.2770359999999998	-4.1608320000000001	3.1082239999999999
H	0.6093130000000001	-4.6638450000000002	3.2706240000000002
C	-1.6660910000000002	-6.6876980000000010	1.0405759999999999
C	-1.6730309999999999	-5.6331009999999999	-0.0707060000000000
C	-0.2994410000000000	-5.0833899999999996	-0.4294400000000000
O	0.7141120000000000	-5.7777979999999998	-0.1702800000000000
O	-0.2650570000000000	-3.9322159999999999	-1.0020290000000001
H	-1.0205530000000000	-7.5312919999999997	0.7774910000000000
H	-2.1006040000000001	-6.0571460000000004	-0.9935050000000000
H	-2.3081630000000000	-4.7841920000000000	0.1947630000000000
C	-6.4203020000000004	-5.8806330000000004	0.3766590000000001
C	-5.1884220000000001	-5.0662740000000008	0.0343350000000000
C	-5.4994459999999998	-3.9314589999999998	-0.9541940000000000
C	-4.2119070000000001	-3.2419840000000000	-1.3424800000000001
O	-3.8747300000000000	-3.1853479999999998	-2.5594820000000000
O	-3.4751290000000004	-2.7988000000000000	-0.3949180000000000
H	-6.1900079999999997	-6.6948330000000000	1.0761210000000001
H	-4.7466280000000003	-4.6337229999999998	0.9381900000000000
H	-4.4274589999999998	-5.7250220000000001	-0.4024300000000000
H	-5.9879190000000007	-4.3229910000000000	-1.8535260000000000
H	-6.1664070000000004	-3.1964359999999998	-0.4869500000000000
C	-5.9465190000000003	-1.7208200000000000	4.9801909999999996
C	-5.1016409999999999	-1.8861730000000001	3.7045610000000000
O	-3.9757180000000001	-0.9684580000000000	3.7102800000000000
C	-5.9302380000000001	-1.7226520000000001	2.4258700000000002
H	-5.3074620000000001	-1.7839480000000003	5.8670549999999997
H	-4.6426069999999999	-2.8842729999999999	3.7169740000000000
H	-4.2727449999999996	-0.0807610000000000	3.3886720000000001
H	-5.3192659999999998	-1.9059560000000000	1.5374300000000001
H	-6.7758099999999999	-2.4231569999999998	2.4192520000000002
H	-6.3172950000000005	-0.7002300000000000	2.3577180000000002
C	-9.8116520000000005	-1.8405540000000000	-0.4754620000000000
C	-8.6158750000000008	-0.8783190000000000	-0.4425720000000000
C	-7.9709709999999996	-0.6700780000000000	-1.8294520000000001
C	-6.5997010000000005	-0.0068160000000000	-1.7239409999999999
O	-5.7544880000000003	-0.4587480000000000	-0.9413060000000000
N	-6.3800970000000001	1.0667679999999999	-2.5099779999999998
H	-10.6067420000000006	-1.4747610000000000	-1.1388750000000001
H	-8.9321850000000005	0.0950470000000000	-0.0419880000000000

H	-7.8462930000000002	-1.2578009999999999	0.2371910000000000
H	-7.8159910000000004	-1.6491720000000001	-2.3047520000000001
H	-8.6431989999999992	-0.0968360000000000	-2.4824220000000001
H	-7.0791380000000004	1.3625710000000000	-3.1711909999999999
H	-5.4747979999999998	1.5504300000000000	-2.5021049999999998
P	0.5860190000000000	-0.0083750000000000	-2.7450380000000001
O	0.2878240000000000	-1.0103180000000000	-1.5783210000000001
O	-0.1820420000000000	1.3207130000000000	-2.5933940000000004
O	1.3771060000000002	-0.5363289999999999	-3.9312879999999999
O	-1.2674510000000001	-0.8559710000000000	-3.8481329999999998
Ca	-0.0325450000000000	-0.0954070000000000	1.7017070000000001
Ca	1.7720180000000001	-2.6600899999999998	-0.6678290000000001
Ca	-1.7555040000000000	-2.1708460000000001	-1.9722299999999999
Fe	-0.5199830000000000	2.3794490000000001	-0.8101350000000000
Fe	2.7340900000000001	1.8068180000000000	0.6797250000000000
O	1.0122300000000000	1.5569459999999999	0.0990850000000000
O	-1.7752950000000001	1.3472059999999999	0.5322730000000000
O	-3.0495169999999998	-0.1018720000000000	-1.3089489999999999
O	-0.8455650000000000	-3.2695390000000000	-4.1447550000000000
O	1.7265740000000001	-3.1227670000000001	-3.2974299999999999
O	3.0515230000000000	-4.7578820000000004	-0.5565840000000000
O	-2.1443669999999999	-1.3896679999999999	1.7517080000000000
H	-6.6574939999999998	3.0366640000000000	3.9771320000000001
H	-7.6997970000000002	3.9694300000000000	2.8765930000000002
H	-5.1694880000000003	6.9393870000000000	-2.8897290000000000
H	-6.8275100000000002	6.3118629999999998	-2.8757259999999998
H	-1.4810470000000000	6.1973979999999997	2.2335420000000004
H	-2.6087600000000002	6.9080360000000010	1.0591150000000000
H	3.0559789999999998	7.8368300000000000	-2.8655080000000002
H	1.7774449999999999	8.3641799999999993	-1.7566590000000000
H	2.4535290000000001	6.0945879999999999	3.5055710000000002
H	4.2101350000000002	5.8651010000000001	3.5790020000000005
H	8.1174040000000005	1.9965459999999999	-0.7258340000000001
H	7.9904299999999999	3.4855360000000002	0.2378560000000000
H	9.4865510000000004	-1.3926310000000000	1.9936900000000000
H	10.3166989999999998	-2.5502250000000002	0.9364749999999999
H	4.7743080000000004	0.5493970000000000	5.6492730000000000
H	6.0995600000000003	-0.0721200000000000	4.6514389999999999
H	0.4888470000000000	-3.5030850000000000	5.5472039999999998
H	1.7525470000000001	-4.7585059999999997	5.5099359999999997
H	-1.2871450000000000	-6.2618739999999997	1.9767589999999999
H	-2.6794669999999998	-7.0635149999999998	1.2257270000000000
H	-7.1946820000000002	-5.2562850000000001	0.8429310000000000
H	-6.8624330000000002	-6.3330900000000003	-0.5214510000000000

H	-6.4433730000000002	-0.7427780000000002	4.9824489999999999
H	-6.7150710000000000	-2.5015749999999999	5.0417030000000000
H	-9.5075760000000002	-2.8317670000000001	-0.8351010000000000
H	-10.2433630000000004	-1.9653750000000001	0.5245310000000000
H	2.2062249999999999	-5.3000590000000001	-0.4224740000000000
H	3.4895090000000000	-4.7204379999999997	0.3041130000000000
H	1.5843970000000001	-2.2097560000000001	-3.6795140000000002
H	0.8986710000000000	-3.5696230000000000	-3.5739800000000002
H	-0.9854710000000000	-2.2564310000000001	-4.3352800000000000
H	-1.5420550000000000	-3.7781970000000005	-4.5753209999999997
H	-3.1175160000000002	0.6724580000000000	-1.9176420000000001
H	-3.9893570000000000	-0.2767010000000000	-1.0589810000000000
H	-2.5038130000000001	2.0316589999999999	0.9803090000000000
H	-2.3309970000000000	0.7429110000000000	-0.0313730000000000
H	-2.7807149999999998	-1.2598790000000000	2.5019710000000002
H	-2.6490260000000001	-1.8873910000000000	1.0843659999999999
C	-1.7683160000000000	0.0955900000000000	-4.7528490000000012
H	-2.6335769999999998	-0.3075840000000000	-5.3082390000000004
H	-2.0944910000000001	1.0068330000000001	-4.2381789999999997
H	-1.0052500000000000	0.3850190000000000	-5.4948090000000001
O	2.1090559999999998	0.6646950000000000	-1.9157910000000000
H	2.4294370000000001	1.5754610000000000	-2.2608600000000001
H	1.6616329999999999	0.9344360000000002	-1.0251729999999999

Prod_{base}

Energy with the medium-sized basis set:	-5579.52383
Solution energy with the medium-sized basis set:	-5579.60687
Energy with larger basis sets:	-5581.62048
Zero-point energy:	1.63512
Dispersion effect:	-0.34808

C	-6.9441130341999999	3.1752560105000001	2.9292670109999999
C	-5.6772876831000003	3.6853379390000001	2.2508224757000002
C	-4.6001661838999999	2.6161517412000004	2.1428748911000000
O	-4.6453254428999999	1.5727648892999999	2.7893059783999998
O	-3.6502682425000001	2.9626203138000000	1.3081464871999999
H	-7.3972511419000000	2.3611902334999999	2.3525807229000004
H	-5.8845730409000003	4.0649363237999996	1.2428396865000000
H	-5.2467419295999997	4.5310697644999998	2.8075807723000006
C	-5.8335688577999996	6.1992948530999996	-2.4251989691000002
C	-5.2754184033000007	4.7750939145000002	-2.5385003584999999
C	-3.8725485372000001	4.7227388221000002	-1.9374197487000000

C	-3.1856340801000003	3.3678709110999998	-1.8709897098000001
O	-3.7568986818000005	2.3179261672000000	-2.2386480946999998
O	-1.9970641417999999	3.4438057812000000	-1.4029764979999999
H	-5.8955816623999997	6.5127489021000002	-1.3751411215000000
H	-5.9317409095000011	4.0672210412999998	-2.0150829763000000
H	-5.2469065669999999	4.4568020440999998	-3.5894318834000001
H	-3.2011032287000001	5.4014497346999999	-2.4826523416000001
H	-3.8957819308000001	5.0972831236000005	-0.9045197260000000
C	-2.0124329410000001	6.0146269622000004	1.2922019861000000
C	-0.8643019040000000	5.7547142969999996	0.3141859873000000
S	0.1425029658000000	4.2783561071999996	0.7885517731000000
H	-2.6951458733000000	5.1614643725000002	1.3177019727999999
H	-1.2469952639999999	5.5872260967000003	-0.6947721873000000
H	-0.1791010504000000	6.6106780382999997	0.2897532083000000
C	2.6654789472000000	7.7270027715999996	-1.8453179823000001
C	2.3328512541999999	6.2212648319000001	-1.8942027071000000
C	3.5826398085000002	5.3263116077000001	-1.6963323580000000
C	3.2414210209999998	3.8387866570000000	-1.6376776563000000
O	3.1958423940000000	3.1694570576999999	-2.6918731242999998
O	3.0203233471000002	3.3589782680000004	-0.4587043904000000
H	3.1062973782000003	8.0002071230999992	-0.8777435669000000
H	1.6044950193000000	5.9770199624000000	-1.1130818032000001
H	1.8642564316000001	5.9708486319000000	-2.8553859868000000
H	4.2821492070999998	5.4842503476999998	-2.5265840064999998
H	4.0800334750999996	5.6057888463000003	-0.7600709671000000
C	3.2520409950000002	5.3420490116000003	3.4634380362999999
C	3.7186485776999998	4.0780372241000000	4.1990910240000003
C	2.5999801574000001	3.0396084977000002	4.3694859273000004
C	2.1827476981000000	2.2342709241000001	3.1345517963999998
O	3.0001640722000000	2.2267928384000002	2.1312606580000000
O	1.1155896617000001	1.5968306847000000	3.2161484738000001
H	2.8833841658999999	5.0942004503999998	2.4616997718000002
H	4.5556016228000002	3.6247384777999998	3.6539947682000000
H	4.0976048597999997	4.3505175329999997	5.1952790987000004
H	2.8860183534999999	2.2907293022999999	5.1224532879000000
H	1.6883584368000000	3.5141604703999998	4.7548068900000002
C	7.5382897282999997	2.5040209058000000	0.0494650121000000
C	6.3047224105000002	2.7959003939999998	-0.8183826765000001
C	5.6751563961000002	1.4534091724000000	-1.1470000526999999
O	6.2293886697999996	0.7386691392000000	-2.0094483862999999
O	4.6848629240999999	1.0649915126000000	-0.4235619395000000
H	7.2505620499000001	1.9959214943000003	0.9778138999000000
H	5.5988280834999999	3.4309365171000006	-0.2787299925000000
H	6.6063301163999997	3.2944666099000002	-1.7459915165000000

C	9.6006388808000001	-1.7184280142999999	0.9539019387000000
C	8.2319061325000007	-1.9399430980000001	0.2870657291000000
C	8.2823214985000000	-2.9802452421000001	-0.8504877950000000
C	6.9065842702999998	-3.3362226012999998	-1.4371188990999999
N	6.3397785468999999	-2.2192525876999998	-2.2019430795999999
C	5.1395526586000004	-2.3001423989999998	-2.8154825799999998
N	4.4615014568000007	-3.4446565308000006	-2.9408993867000000
N	4.6531531437000000	-1.1803779388000002	-3.3840356405000001
H	10.3410091233999992	-1.3572421971999999	0.2282665093000000
H	7.5049269097000000	-2.2767320543000000	1.0389341217000001
H	7.8549576776999999	-0.9812156245000000	-0.0944209723000000
H	8.9410255811999999	-2.6275938829999999	-1.6573424656000000
H	8.7288274065000007	-3.9077840116000000	-0.4639392690000000
H	7.0084907250999997	-4.1969328160000003	-2.1112473414999999
H	6.2280965477999999	-3.6250065258999999	-0.6205743419999999
H	6.6133888464000004	-1.2654594260000003	-1.9649637771999999
H	4.6755409987999998	-4.1814451367999999	-2.2815312318000003
H	3.3987983993999999	-3.2759654159000000	-3.0974368279000002
H	5.0588729173999996	-0.3044528476000000	-3.0468682204999999
H	3.6596878516000002	-1.1783457953000001	-3.5777632493999998
C	5.1090530319000003	0.4018700791000000	4.6151140451000003
C	4.3046928107999998	-0.5125333793000000	3.6737933729000001
C	4.9109085226999998	-0.5301714577000000	2.2475276636000001
C	3.9826792539999998	-1.1361869838000000	1.2089917915999999
O	4.1647034364000000	-2.2933805463999999	0.7722158296000000
O	2.9556663150000002	-0.4466145161000000	0.8158123048000000
H	5.1237510900999998	1.4286313820000001	4.2362009872000002
H	4.2804090032000000	-1.5348669983000001	4.0750395678000002
H	3.2651318508000000	-0.1736552049000000	3.6274351161000000
H	5.1309393997999999	0.4984441166000000	1.9466759350000000
H	5.8493209291000001	-1.0947162839000000	2.2499402927999999
C	1.4436530348000001	-3.7905259797000004	5.0971330682999998
C	1.5440196975000000	-3.6308946318999999	3.5727903947000001
C	0.9159440025000000	-2.3453950287000001	3.0388430167000000
O	0.3975862435000000	-1.5254592843999999	3.8434822944999998
O	0.9460272303000001	-2.1362119152000001	1.7715163294000000
H	1.9426549990999999	-2.9620101321000001	5.6104256384999998
H	2.5960213266999999	-3.6372645942999999	3.2496158429000004
H	1.0716690372000000	-4.4702156868999996	3.0445806200000001
C	-1.6660908498000000	-6.6876976933000005	1.0405758357999999
C	-1.6380668952999999	-5.3898507042999997	0.2294536296000000
C	-0.2559340625000000	-4.7798228678000001	0.0269166614000000
O	0.7446452917000000	-5.3833837534000004	0.4877859670000000
O	-0.2014761733000000	-3.6741631587999999	-0.6280922269000001

H	-1.0492311349000001	-7.4618132233000001	0.5715096935000001
H	-2.0697548219000002	-5.5504290456999996	-0.7697372186000000
H	-2.2656767564000000	-4.6177727615000004	0.6862582332000000
C	-6.4203019625000000	-5.8806329445000003	0.3766590031000000
C	-5.1251618626999997	-5.1511629764000002	0.0168078367000000
C	-5.3528847342999999	-3.9505068120000000	-0.9241882268000001
C	-4.0350410882999999	-3.2862910715000000	-1.3036763727000000
O	-3.6424183184999999	-3.3451764278999998	-2.5035501299999998
O	-3.3476358281000000	-2.7293854683999998	-0.3829713071000000
H	-6.2307204973000001	-6.7280010063000004	1.0478747299000000
H	-4.6288294725999997	-4.7963921425000002	0.9278303056000000
H	-4.4345918066000003	-5.8576360625000001	-0.4621139051000000
H	-5.8583786303999998	-4.2793327747000012	-1.8396124650000001
H	-5.9847381482999999	-3.2052189180999999	-0.4257584976000001
C	-5.9465190030999997	-1.7208199919000000	4.9801910019999998
C	-5.0987356441999996	-1.8953651522999999	3.7178769148000002
O	-3.9876866204999999	-0.9548639345000000	3.7370833222000002
C	-5.9054445750999998	-1.7505565366000000	2.4247296620999998
H	-5.3202467009000003	-1.8082451709000003	5.8737921386999998
H	-4.6161756293999998	-2.8806164163000001	3.7418980540000000
H	-4.3056443206999999	-0.0736984182000000	3.4521669479999999
H	-5.2717119788000000	-1.8973814816000001	1.5457124946000000
H	-6.7204197906000003	-2.4848549267000002	2.3935324215000002
H	-6.3425350355000001	-0.7469960723000000	2.3587238269999999
C	-9.8116519697999998	-1.8405539804000000	-0.4754620071000000
C	-8.5496781003999995	-0.9637022487000001	-0.4106010397000000
C	-7.8754790966000012	-0.7649645327000000	-1.7861842172000000
C	-6.5178507388000000	-0.0711452934000000	-1.6628604812000001
O	-5.6622568645999998	-0.5067332986999999	-0.8835400134000000
N	-6.3201833849000000	1.0189806361000000	-2.4373641328000000
H	-10.5724601373000020	-1.4022725903000002	-1.1345676871999999
H	-8.8013018118000002	0.0190799258000000	0.0134553777000000
H	-7.8153997074000001	-1.4139004207000001	0.2652378033000000
H	-7.6912553601000004	-1.7486113259000002	-2.2405855730000006
H	-8.5450287038999999	-0.2165918264000000	-2.4631071658999999
H	-7.0300097600000004	1.3218494026000001	-3.0842465127000005
H	-5.4334731698000001	1.5323064997000000	-2.4026438671000001
P	0.8598540717000001	0.4486492166000000	-2.4535688304000001
O	0.4473007840000000	-0.6517400515000000	-1.3971820280000000
O	-0.0229287133000000	1.7096876861000001	-2.2277874490000000
O	0.8978220267000000	-0.0808572900000000	-3.8707376465999999
O	-1.5918456325000001	-0.8817738481000000	-4.2144104220000003
Ca	-0.3027191797000000	0.0256374633000000	2.1190681245000000
Ca	1.8936129765000000	-2.4378236818999999	-0.4913605810000000

Ca	-1.5416086981000001	-2.1412668676000002	-2.0946415482999998
Fe	-0.5984628980000000	2.4388234490000000	-0.4733959648000000
Fe	2.8620729934000004	1.5322269543000000	0.2700065795000000
O	0.9057807342999999	1.2502893991999999	0.3617419700000000
O	-1.8035367605999999	1.3736036706999999	0.7220930491000001
O	-2.9069453780000001	-0.1279434185000000	-1.3646914021000001
O	-0.2862554437000000	-3.7663382689999998	-3.4936463188000002
O	1.9953818441000000	-2.7178082249000002	-2.9027817594999998
O	3.1026916889999998	-4.6304425532000000	-0.3264642287000000
O	-2.1897859295000002	-1.4640633215000001	1.8209013437999999
H	-6.7188760760999999	2.7823102664000001	3.9255008243999998
H	-7.6859407196999996	3.9758758271999999	3.0312959112000000
H	-5.1875426065000001	6.9175887340999997	-2.9463136999000001
H	-6.8388487451000000	6.2815716551999996	-2.8575422206000001
H	-1.6329561375999999	6.1748345853000002	2.3086086485999999
H	-2.5753244333000005	6.9122769871000003	0.9946070740000000
H	3.3821769770999999	8.0025567745000004	-2.6304531734999999
H	1.7618250192000000	8.3320264113999993	-1.9870490949000001
H	2.4351620379000001	5.8349414801000004	4.0080610073000003
H	4.0705144783999998	6.0659313049000003	3.3583148725000003
H	8.2403014904000003	1.8602764985000000	-0.4911708417000000
H	8.0621355239000003	3.4277588991000005	0.3234991611000000
H	9.5331883174000023	-0.9777962692000000	1.7591073793000001
H	9.9853212603999992	-2.6515192509999999	1.3864699326000001
H	4.6764229093000003	0.4135589255000000	5.6227890907999996
H	6.1497044999000003	0.0615061727000000	4.7033594190999999
H	0.3973045359000000	-3.7887649831000001	5.4192384643000002
H	1.9061312339000001	-4.7316916762999996	5.4205313965000013
H	-1.2713995025000000	-6.5264045829999997	2.0493720092999999
H	-2.6914561297000001	-7.0672025766999997	1.1290139626000000
H	-7.1280664666000000	-5.2082057686000001	0.8803615269000000
H	-6.9184450982000003	-6.2710210451000004	-0.5209703042000000
H	-6.4198886608999999	-0.7309690470000000	4.9869467226999999
H	-6.7371662644999999	-2.4797613614000005	5.0300625690000000
H	-9.5745216286999995	-2.8410124305000002	-0.8585828340000000
H	-10.2582566129000003	-1.9592833811999999	0.5185486491000000
H	2.2718080055000001	-5.0754006703000005	0.0182592454000000
H	3.6538598340999999	-4.4244238869999997	0.4412950253000000
H	1.7480787913000002	-1.9522317910000000	-3.4490551550999999
H	0.6800112573000000	-3.4816975236999999	-3.3245346511000000
H	-0.6682704315000000	-0.5332737415000000	-4.3224160256999999
H	-0.3545144321000000	-4.6282816143999996	-3.0668044249999999
H	-3.0490344791999999	0.7349171936000000	-1.8226508908000001
H	-3.8094089786000005	-0.3909826233000000	-1.0780340501000001

H	-2.8901566590000001	2.2550749266999999	1.1642052264000000
H	-2.2712367976999999	0.7420883181000000	0.1270440629000000
H	-2.8889171923000005	-1.3529100297000001	2.5095918964999999
H	-2.6089934509999999	-1.9334023654000003	1.0736141559000001
C	-2.5258718848999999	0.0438728661000000	-4.7570978891999998
H	-2.3733783708999998	0.1694740069000000	-5.8372266141000004
H	-3.5283608389999999	-0.3628747068000000	-4.5959536543999997
H	-2.4621917880000002	1.0238835634000001	-4.2692689170999998
O	2.3769541363000002	0.8560283353000000	-1.9753900034000000
H	2.7070587185999999	1.7363779277000000	-2.3924966723000001
H	0.7643061085000000	0.4446908746000000	-0.2095400134000000

Enzyme-methyl phosphate complex indicated in entry 2 of Table S1

Energy with the medium-sized basis set:	-5503.04278
Solution energy with the medium-sized basis set:	-5503.12611
Energy with larger basis sets:	-5505.08391
Zero-point energy:	1.60996
Dispersion effect:	-0.33791

C	-6.8650001836	-6.1059998972	20.3889998943
C	-7.6283225737	-5.0602304416	19.5725089902
C	-9.1202362559	-5.4027928384	19.3790175685
O	-9.4420868666	-6.6135718581	19.4517545183
O	-9.8711634450	-4.4064284130	19.1344423344
H	-7.2533266102	-6.1628530460	21.4135794373
H	-7.5590829227	-4.0664981632	20.0316323237
H	-7.1831356007	-4.9661575020	18.5695670780
C	-7.4140001011	-0.0290000426	21.7369999666
C	-8.7844907861	-0.6999286724	21.9343875359
C	-9.4794447089	-0.9609497622	20.5919535141
C	-10.9018172425	-1.5190284320	20.6484624053
O	-11.3108050820	-2.0917299273	21.6927189607
O	-11.5719914984	-1.3475541547	19.5799862969
H	-6.7555560840	-0.6570319846	21.1232829557
H	-8.6576731333	-1.6489787421	22.4710053317
H	-9.4238336554	-0.0662964445	22.5650039184
H	-9.5106968304	-0.0387762136	19.9974860702
H	-8.8987286011	-1.6869512401	20.0042875164
C	-8.8830000589	-1.7600000020	16.9099999749
C	-10.2062074928	-1.0166585887	16.7107104766
S	-11.5662742014	-2.1814389355	16.3416667984
H	-8.9890011904	-2.5316328916	17.6792465651

H	-10.4953034124	-0.5079610875	17.6369388035
H	-10.1280374368	-0.2739741743	15.9104761863
C	-11.9689999871	2.8629998900	14.9700000969
C	-12.3659926409	1.5440536664	15.6379733539
C	-13.8475645742	1.4779776665	16.0703926386
C	-14.1596319384	0.0840999554	16.6229667573
O	-13.5326146081	-0.2469422199	17.6735952304
O	-14.9694943651	-0.6269630635	15.9632887085
H	-12.5560713768	3.0422973742	14.0592480508
H	-12.1648093210	0.7099870923	14.9524380311
H	-11.7472578389	1.3743020724	16.5249551891
H	-14.0357749534	2.2283994319	16.8511513318
H	-14.5088729319	1.6881902444	15.2223150268
C	-12.1639999333	-2.3060000031	12.2389999731
C	-13.3116897593	-3.3181658736	12.1255095214
C	-13.1975699326	-4.4398122815	13.1689036640
C	-13.8295510303	-4.2150719997	14.5538456764
O	-14.6675539710	-3.2543487851	14.6921012154
O	-13.4953733919	-5.0563654577	15.4206471731
H	-12.1438110706	-1.8601772128	13.2400827600
H	-14.2717765673	-2.8037208117	12.2518166620
H	-13.3119022902	-3.7564878365	11.1164436819
H	-13.6477506573	-5.3673200913	12.7926213679
H	-12.1439309100	-4.6855106526	13.3537404313
C	-18.0649999587	-0.5230001191	12.5230002001
C	-17.2022707143	-1.0097899540	13.6838469662
C	-18.0260199617	-1.6307488334	14.7921490274
O	-19.2792431437	-1.5277009276	14.7614827649
O	-17.4192391243	-2.2524012260	15.7343320715
H	-18.6252516669	-1.3496640713	12.0718637444
H	-16.4526973863	-1.7438908603	13.3625455435
H	-16.6152411806	-0.1974569429	14.1315738157
C	-21.9319999590	-3.3250000089	12.2140001621
C	-21.7442022803	-3.6600975704	13.7020237846
C	-22.4461353781	-2.6391593434	14.6166866744
C	-22.2657092478	-2.9138133001	16.1185901913
N	-20.8663887163	-2.7140034280	16.5189413742
C	-20.4195172008	-2.9393499208	17.7384473808
N	-21.2300498671	-3.2568907533	18.7669375319
N	-19.0758356337	-2.8676420156	17.9938022966
H	-21.4983785801	-2.3449918824	11.9814056088
H	-22.1338034759	-4.6672002581	13.9125341600
H	-20.6732256271	-3.6793125093	13.9337127687
H	-22.0688893665	-1.6325341259	14.3934130378

H	-23.5243894872	-2.6322230283	14.4021809788
H	-22.9169852692	-2.2377362651	16.6943481247
H	-22.5687190299	-3.9468042380	16.3473113175
H	-20.1895960471	-2.2722287566	15.8207417664
H	-22.2039526968	-3.4316626347	18.5793245441
H	-20.8074612602	-3.7423869692	19.5676525749
H	-18.4667110033	-2.5655649234	17.2095034531
H	-18.8235808470	-2.3869491083	18.8525309058
C	-16.2809998664	-5.8030000417	12.1999997639
C	-16.5143913410	-6.1665649051	13.6799327356
C	-17.3396476087	-5.0617696637	14.3817707150
C	-17.4560867307	-5.2086704191	15.8910245772
O	-18.4548223019	-5.8030048782	16.3800600262
O	-16.5463666727	-4.7044185731	16.6576750587
H	-15.7952565682	-4.8271636715	12.1092143069
H	-17.0380082259	-7.1297607579	13.7526042031
H	-15.5557906780	-6.2913752584	14.1950157445
H	-16.8583863374	-4.1064114542	14.1718480172
H	-18.3545991855	-5.0494541682	13.9653898871
C	-16.3929999507	-9.8490000267	16.0549999484
C	-16.6767227914	-9.1129667527	17.3702181913
C	-15.8343748233	-7.8477761695	17.5404060677
O	-14.7968743532	-7.7204715435	16.8460075444
O	-16.2216607902	-6.9743476209	18.3966205567
H	-16.6277931654	-9.2120154141	15.1958023394
H	-17.7365537662	-8.8367934116	17.4511837875
H	-16.4636155758	-9.7660728566	18.2305302719
C	-17.5420000277	-9.6659997082	21.8140000256
C	-17.2688781941	-8.2226473320	22.2707440782
C	-17.9936743338	-7.1326825480	21.4936289488
O	-19.2263297557	-7.2615887316	21.2242307165
O	-17.3301467103	-6.0865284779	21.1717365747
H	-18.6129306385	-9.8934602476	21.8463145011
H	-17.5773677263	-8.1119795595	23.3220526818
H	-16.2022817926	-8.0036712549	22.2209700926
C	-14.0159999779	-9.9710000239	25.1559999562
C	-14.5578412818	-8.8361432877	24.3062229746
C	-13.8635886929	-7.4914162693	24.5871219019
C	-14.3934762826	-6.4448516173	23.6293978948
O	-15.0005481308	-5.4254502502	24.0726055672
O	-14.2644358975	-6.6828473070	22.3787632326
H	-14.5223391272	-10.9198567278	24.9357830273
H	-14.4297671234	-9.0710121929	23.2440590602
H	-15.6356599996	-8.7299290064	24.4839478958

H	-14.0316034138	-7.1694427389	25.6208227866
H	-12.7842667901	-7.5900864394	24.4227685858
C	-10.0720000148	-10.4519999802	20.3670000208
C	-11.1217089584	-9.3650328041	20.6543450777
O	-11.3001331565	-8.5094762253	19.4978242314
C	-10.7836992211	-8.5378654267	21.8997326314
H	-10.3416452219	-11.0098621801	19.4639965169
H	-12.0980605249	-9.8504032109	20.7938612932
H	-10.5877348363	-7.8131958034	19.4751454553
H	-11.5628056496	-7.7967873749	22.1008805892
H	-10.6818599214	-9.1867084827	22.7799245831
H	-9.8413146504	-7.9999114916	21.7481488078
C	-9.3519999809	-7.6870000363	26.4130000272
C	-9.6348160905	-6.8655796362	25.1437616760
C	-10.1815468319	-5.4520599453	25.4396559313
C	-10.7084130186	-4.7623579239	24.1795185959
O	-11.4955842589	-5.3604220064	23.4331740601
N	-10.2933307122	-3.5003814538	23.9522013290
H	-8.6066721155	-7.1969165872	27.0534292173
H	-8.7194351896	-6.7808533780	24.5418272127
H	-10.3654901274	-7.3868136820	24.5178175375
H	-11.0310377638	-5.5347888102	26.1333754462
H	-9.4169071009	-4.8411298028	25.9391576020
H	-9.6473420322	-3.0581521872	24.5855802061
H	-10.6027793318	-2.9748915472	23.1213839937
P	-15.9933067561	-2.2773636161	19.5292687679
O	-16.4594719565	-3.7137312193	19.8975867704
O	-14.5629718192	-2.0155118870	19.9754385679
O	-16.4609972438	-1.8317655543	18.1451858177
O	-16.9745932311	-1.3695612798	20.5752682525
Ca	-14.0512156265	-5.5668632558	17.6550874025
Ca	-17.8394577689	-5.2806257906	18.7501184214
Ca	-15.4432852883	-4.6675703465	21.8077333794
Fe	-13.0337737325	-2.1488191954	18.4508509579
Fe	-15.5468694329	-2.5999903463	16.4351771670
O	-14.3003839597	-3.2063847956	17.4091124493
O	-12.3915491568	-4.2503398499	19.0148487771
O	-13.1254331047	-4.0359921538	21.6893229464
O	-16.7287077335	-2.8445635450	22.8172954939
O	-19.6636600503	-4.6363008758	20.6463928771
O	-19.8312338091	-6.7791312920	18.6474865562
O	-13.4689199496	-6.9454778955	19.6475722849
H	-6.9901909952	-7.0956256705	19.9403308095
H	-5.7931647557	-5.8726994321	20.4450122646

H	-7.5196723420	0.9371153131	21.2266872640
H	-6.9085173794	0.1511744186	22.6945150622
H	-8.5600290211	-2.2508064800	15.9834521105
H	-8.0922689656	-1.0570493430	17.2088842102
H	-12.1333311698	3.7163576280	15.6422844977
H	-10.9085439103	2.8609061020	14.6873934215
H	-11.1946944228	-2.7941275109	12.0699627896
H	-12.2644376044	-1.4947906832	11.5057331385
H	-18.7952485289	0.2192857567	12.8600519864
H	-17.4446592766	-0.0663464517	11.7416777371
H	-21.4395647784	-4.0680771584	11.5765525882
H	-22.9953691440	-3.2990993949	11.9399784430
H	-15.6508923487	-6.5477567893	11.6980260055
H	-17.2345395435	-5.7518513087	11.6559279733
H	-15.3339825857	-10.1108256005	15.9872170154
H	-16.9908085032	-10.7661532301	15.9787228431
H	-17.1906390644	-9.8223731846	20.7874429694
H	-17.0152250029	-10.3755464963	22.4615204849
H	-12.9426760320	-10.1212286852	24.9782511991
H	-14.1450409629	-9.7692250705	26.2283295003
H	-9.0893218390	-9.9919545648	20.2059796558
H	-9.9948417036	-11.1541177388	21.2071241380
H	-10.2658345575	-7.8201006017	27.0062848653
H	-8.9701141906	-8.6821677831	26.1573563259
H	-19.7560114960	-7.3419876788	19.4448805641
H	-19.6838583125	-7.3069904457	17.8517191006
H	-19.0779068121	-4.2258427330	21.2986272200
H	-19.6745571489	-5.6005210176	20.9084421281
H	-16.8708165432	-2.1584511364	22.1182622436
H	-16.3780021070	-2.4031860342	23.5995975954
H	-12.6549964600	-3.1616449674	21.6325386408
H	-12.5279234373	-4.5925251921	22.2473781596
H	-11.3599721110	-4.3810409466	18.9879662487
H	-12.6116727508	-4.3464593965	19.9676839150
H	-12.6628527045	-7.5258375295	19.5853959591
H	-13.7358727442	-6.9961313230	20.5807572671
C	-16.7575489487	0.0526967908	20.5459162560
H	-17.4108471137	0.4965219233	21.3025526703
H	-15.7106223853	0.2843905010	20.7673055498
H	-17.0143809652	0.4489987932	19.5590366263

Enzyme-methyl phosphate complex indicated in entry 3 of Table S1

Energy with the medium-sized basis set:	-5503.02400
Solution energy with the medium-sized basis set:	-5503.11078
Energy with larger basis sets:	-5505.06494
Zero-point energy:	1.61261
Dispersion effect:	-0.33270

C	-6.8650002208	-6.1059998821	20.3889998862
C	-7.6274639430	-5.0773085666	19.5499046914
C	-9.1211811247	-5.4200191726	19.4026394950
O	-9.4191173217	-6.6342510879	19.2783603097
O	-9.8995503990	-4.4165216008	19.4012371919
H	-7.2321427103	-6.1190203892	21.4237053213
H	-7.5402437132	-4.0700272735	19.9718308281
H	-7.2014667874	-5.0338570893	18.5357436858
C	-7.4140000339	-0.0290000093	21.7369999932
C	-8.6762512929	-0.9101130178	21.7302365701
C	-9.6323427177	-0.5546738307	20.5821313230
C	-10.8817545706	-1.4419427752	20.4516651055
O	-11.2717831223	-2.0864256011	21.4674495957
O	-11.4316376613	-1.3821356678	19.3119775289
H	-6.8560313749	-0.1386069147	20.7986078136
H	-8.3869019455	-1.9657312546	21.6370885873
H	-9.2075142502	-0.8105919726	22.6867381879
H	-9.9839467559	0.4833709386	20.6975725647
H	-9.1046675381	-0.5913390474	19.6226513778
C	-8.8830000248	-1.7600000358	16.9100000158
C	-10.2729421397	-1.3243914204	16.4654326011
S	-11.4523079819	-2.7347012535	16.4408450749
H	-8.9370915490	-2.2581105165	17.8826118165
H	-10.6756512912	-0.5791708661	17.1536124508
H	-10.2398078984	-0.8856554089	15.4598714604
C	-11.9690000075	2.8629998855	14.9700001044
C	-12.2296021816	1.4507769950	15.5271233771
C	-13.6841628609	1.2089665471	15.9966989251
C	-13.8926266927	-0.2102304496	16.5437510958
O	-13.2090136660	-0.5263911498	17.5557652044
O	-14.7355900132	-0.9280228901	15.9243666244
H	-12.6037424713	3.0740270229	14.0990011638
H	-11.9788288056	0.7062610986	14.7600280715
H	-11.5598092655	1.2619222696	16.3717028758
H	-13.9280729433	1.9197838294	16.7996550657
H	-14.3875169181	1.3748316872	15.1730485837
C	-12.1639999334	-2.3060000266	12.2389999954
C	-13.2883549590	-3.3462241302	12.1383437623

C	-13.1392809306	-4.4697523697	13.1781961728
C	-13.8184139594	-4.2990482385	14.5447631505
O	-14.6217713958	-3.3038990992	14.6964801208
O	-13.5694870295	-5.1973159790	15.3757685119
H	-12.1324066803	-1.8781232969	13.2477120482
H	-14.2583694192	-2.8532911769	12.2746707460
H	-13.2893365369	-3.7825199114	11.1283083727
H	-13.5181169946	-5.4211365142	12.7826615923
H	-12.0791386391	-4.6486967371	13.3996439896
C	-18.0649999658	-0.5230001120	12.5230001812
C	-17.1778161359	-0.8165101826	13.7317294408
C	-17.9660446638	-1.4649967656	14.8545927980
O	-19.2176566663	-1.2872810299	14.8858315593
O	-17.3520427991	-2.1702844118	15.7167241448
H	-18.4869773435	-1.4473730024	12.1107962465
H	-16.3293010592	-1.4616802610	13.4801194616
H	-16.7323541035	0.1058212782	14.1297600701
C	-21.9319999626	-3.3250000091	12.2140001556
C	-21.6244247171	-3.5865270995	13.6996357511
C	-22.3303780887	-2.5802547587	14.6284871575
C	-22.1281639886	-2.8496861790	16.1301519272
N	-20.7304058267	-2.6319852618	16.5282237075
C	-20.2833388549	-2.8610953952	17.7459330140
N	-21.0892922212	-3.2015027314	18.7712005991
N	-18.9370579074	-2.7728845000	18.0044866999
H	-21.5963378272	-2.3235485928	11.9178340838
H	-21.9310612914	-4.6084886629	13.9679672729
H	-20.5418073189	-3.5279677539	13.8622405281
H	-21.9793955325	-1.5656719405	14.3987447692
H	-23.4122369225	-2.5973526327	14.4320822640
H	-22.7881391378	-2.1827786287	16.7075010938
H	-22.4161368255	-3.8863472679	16.3618427795
H	-20.0688637497	-2.1147231405	15.8484587148
H	-22.0620203730	-3.3791394504	18.5795892279
H	-20.6665112706	-3.7060598923	19.5595518009
H	-18.3336897067	-2.4728532688	17.2110166950
H	-18.6941806276	-2.2765800188	18.8570251503
C	-16.2809998639	-5.8030000419	12.1999997734
C	-16.5276835175	-6.0972702201	13.6903321802
C	-17.2230073372	-4.8922604911	14.3716847853
C	-17.2996714002	-5.0183842411	15.8803120105
O	-18.2433762248	-5.6748660319	16.3876841163
O	-16.4066863025	-4.4763613205	16.6561694101
H	-15.6973525958	-4.8870397512	12.0722660559

H	-17.1489816734	-6.9963371285	13.8018674985
H	-15.5776941202	-6.3057703864	14.1938066818
H	-16.6760659569	-3.9884142744	14.1120096982
H	-18.2504547157	-4.8093689871	13.9956398020
C	-16.3929999576	-9.8490000276	16.0549999509
C	-16.6751385892	-9.0441150522	17.3321433958
C	-15.7623789542	-7.8266808804	17.5039706871
O	-14.6873049677	-7.7796288120	16.8605896801
O	-16.1336227446	-6.9054185357	18.3185594981
H	-16.5613737449	-9.2345676630	15.1641754853
H	-17.7171741908	-8.6986977224	17.3596124255
H	-16.5397996135	-9.6780721985	18.2221967761
C	-17.5420000426	-9.6659997414	21.8140000286
C	-17.0657104822	-8.2277860736	22.0638358017
C	-17.8303329418	-7.1125858680	21.3664620932
O	-19.0515350153	-7.2551671895	21.0684820996
O	-17.1985101468	-6.0170599987	21.1435381874
H	-18.6019570402	-9.7809070919	22.0645942480
H	-17.1345792605	-8.0012644623	23.1388279148
H	-16.0108978714	-8.1099326173	21.8057060444
C	-14.0159999919	-9.9710000415	25.1559999688
C	-14.5796020874	-8.8085913874	24.3566959348
C	-13.8685623144	-7.4739319377	24.6479602489
C	-14.3741575259	-6.4161063409	23.6886767286
O	-15.0242637023	-5.4187103481	24.1242871209
O	-14.1799471290	-6.6219236792	22.4426497505
H	-14.5392141897	-10.9090486637	24.9295894598
H	-14.4868681976	-9.0175907638	23.2858301604
H	-15.6510723814	-8.7017764151	24.5723410384
H	-14.0369883833	-7.1550384391	25.6822920392
H	-12.7906687989	-7.5889242647	24.4878014566
C	-10.0720000086	-10.4519999847	20.3670000092
C	-11.0784987510	-9.3327467004	20.6738686347
O	-11.2812266485	-8.4992852131	19.5055001424
C	-10.6676469785	-8.4885088870	21.8845727263
H	-10.3943925363	-11.0210079078	19.4886410992
H	-12.0607175948	-9.7879982288	20.8646923429
H	-10.5595092137	-7.8121335236	19.4375132670
H	-11.4199308750	-7.7258696192	22.1070067724
H	-10.5400454118	-9.1212529191	22.7725176016
H	-9.7201638129	-7.9771909626	21.6800897879
C	-9.3519999865	-7.6869999835	26.4129999475
C	-9.6666561801	-6.9384004262	25.1032968941
C	-9.9385730506	-5.4294368959	25.2934313280

C	-10.5529577556	-4.7797419764	24.0472231733
O	-11.5014513707	-5.3265798396	23.4679329341
N	-10.0427310534	-3.5948811239	23.6570877008
H	-8.4582045996	-7.2821422742	26.9057800116
H	-8.8391803943	-7.0684451063	24.3925433053
H	-10.5480546040	-7.3805888981	24.6297077157
H	-10.6692147650	-5.2968720196	26.1055376995
H	-9.0216708182	-4.9080258212	25.6011885390
H	-9.2455110288	-3.2017892365	24.1302905492
H	-10.4172455087	-3.0886628535	22.8432440012
P	-15.6824911098	-2.2543673054	19.4078025538
O	-16.2056682451	-3.6402035607	19.8799310431
O	-14.2195133960	-2.0090665983	19.7508082246
O	-16.2279883210	-1.8529037607	18.0316240677
O	-16.5459172827	-1.2447251252	20.4570661520
Ca	-13.8671048264	-5.6310055503	17.6717840252
Ca	-17.6652281729	-5.1551193469	18.7597055597
Ca	-15.3604204780	-4.6126258704	21.8592397316
Fe	-12.8237952847	-2.3359732744	18.2365464981
Fe	-15.4132675559	-2.6752435827	16.3741655382
O	-14.1290321180	-3.3051173709	17.3913188725
O	-12.3325874063	-4.1671633302	19.0198639151
O	-13.0716853435	-3.9541755872	21.6914192295
O	-16.4827578744	-2.6347196089	22.7617404242
O	-19.5541668910	-4.6162599443	20.6423313193
O	-19.7073624824	-6.6087151476	18.5195388573
O	-13.3956352470	-6.9274599599	19.7142985601
H	-7.0150067663	-7.1069707585	19.9740009712
H	-5.7883157245	-5.8911917046	20.4174519466
H	-7.6731921153	1.0325332403	21.8464113264
H	-6.7395950360	-0.2962383373	22.5607190051
H	-8.4474033797	-2.4760777533	16.2014355160
H	-8.1982414349	-0.8991964774	16.9825248814
H	-12.1748976188	3.6325182784	15.7262398223
H	-10.9232727655	2.9703836989	14.6575020302
H	-11.1864384570	-2.7663597720	12.0437857428
H	-12.3026685186	-1.4880898826	11.5196132774
H	-18.9021234516	0.1225096056	12.8028589982
H	-17.4941763508	-0.0299293706	11.7258415775
H	-21.4216007997	-4.0516981420	11.5718787435
H	-23.0091477417	-3.3939597738	12.0112116498
H	-15.7375927831	-6.6235265796	11.7150429497
H	-17.2311765025	-5.6693712775	11.6640051833
H	-15.3498463188	-10.1751785588	16.0344082781

H	-17.0423040561	-10.7313569005	15.9948276452
H	-17.4142898133	-9.9452008930	20.7614117082
H	-16.9606195884	-10.3685319986	22.4212653286
H	-12.9518064705	-10.1242622274	24.9327571907
H	-14.1022557128	-9.7971111379	26.2373543388
H	-9.0852015125	-10.0228896958	20.1541027349
H	-9.9770715119	-11.1385555275	21.2181061893
H	-10.1877888161	-7.6091882718	27.1202511620
H	-9.1738678682	-8.7508318482	26.2185516253
H	-19.6209923673	-7.2574994478	19.2436830308
H	-19.4954213822	-7.0274138799	17.6732815429
H	-19.0278200756	-4.2331902257	21.3575818996
H	-19.5439973735	-5.5967217759	20.8385749602
H	-16.5507309663	-1.9864869551	22.0152375836
H	-16.0742329426	-2.1774528456	23.5062717921
H	-12.5471251349	-3.1077912899	21.5598810963
H	-12.4846452784	-4.5266333442	22.2439472776
H	-11.2785861055	-4.3314988325	19.0994842111
H	-12.6230541415	-4.1811484009	19.9613376682
H	-12.6080631628	-7.5368385661	19.6467090732
H	-13.6122980679	-6.9030082223	20.6618181242
C	-16.2353984258	0.1574901795	20.3725178490
H	-16.8180605771	0.6657478577	21.1461580831
H	-15.1651932314	0.3211514761	20.5332929215
H	-16.5184575595	0.5432981530	19.3883097203

Enzyme-methyl phosphate complex indicated in entry 4 of Table S1

Energy with the medium-sized basis set:	-5503.02341
Solution energy with the medium-sized basis set:	-5503.11090
Energy with larger basis sets:	-5505.06475
Zero-point energy:	1.61275
Dispersion effect:	-0.33244

C	-6.8650002122	-6.1059998855	20.3889998883
C	-7.6262975774	-5.0779294649	19.5478850699
C	-9.1211883233	-5.4168052737	19.4044455177
O	-9.4229875109	-6.6297178940	19.2786684434
O	-9.8971253064	-4.4112129972	19.4074342891
H	-7.2304954470	-6.1152771162	21.4243095008
H	-7.5352493825	-4.0694788253	19.9661294375
H	-7.2022831908	-5.0394445170	18.5326894204
C	-7.4140000623	-0.0290000425	21.7369999966

C	-8.6762575143	-0.9093223236	21.7367003126
C	-9.6450133572	-0.5390006566	20.6039776626
C	-10.8868958522	-1.4350296814	20.4670606579
O	-11.2819128353	-2.0757642751	21.4839762930
O	-11.4241209771	-1.3878862209	19.3216801653
H	-6.8682414432	-0.1287868451	20.7903826695
H	-8.3893886857	-1.9641101342	21.6285650834
H	-9.1956443070	-0.8197837970	22.7006834297
H	-10.0039465502	0.4935981510	20.7437300202
H	-9.1250409548	-0.5526481012	19.6397097777
C	-8.8830000164	-1.7600000336	16.9100000125
C	-10.2762192623	-1.3328110928	16.4662776360
S	-11.4527728259	-2.7463500165	16.4580893734
H	-8.9322072551	-2.2484805196	17.8877238409
H	-10.6783289354	-0.5830547692	17.1497012521
H	-10.2483514464	-0.9030290599	15.4567257732
C	-11.9690000072	2.8629998885	14.9700001048
C	-12.2285123448	1.4499487488	15.5253272056
C	-13.6795465031	1.2110176507	16.0077232333
C	-13.8861786396	-0.2095232586	16.5514493522
O	-13.1991443531	-0.5270854766	17.5615836706
O	-14.7256001148	-0.9285373160	15.9294732075
H	-12.6113439738	3.0785527069	14.1057240818
H	-11.9871832038	0.7069332774	14.7536585829
H	-11.5512645470	1.2570574064	16.3629959842
H	-13.9137653047	1.9198169054	16.8151822817
H	-14.3898814411	1.3811678452	15.1910101680
C	-12.1639999323	-2.3060000233	12.2389999921
C	-13.2807734431	-3.3550235631	12.1419379527
C	-13.1292048474	-4.4733168322	13.1876911073
C	-13.8160058872	-4.3043149512	14.5509397482
O	-14.6134187022	-3.3042949184	14.7019300961
O	-13.5771858956	-5.2078970826	15.3792601964
H	-12.1429775031	-1.8660681456	13.2427639239
H	-14.2543164046	-2.8673737875	12.2719828567
H	-13.2754039026	-3.7969964417	11.1343684428
H	-13.4998498167	-5.4285402091	12.7934718849
H	-12.0688280644	-4.6447833812	13.4144486531
C	-18.0649999660	-0.5230001094	12.5230001811
C	-17.1772026727	-0.8080109611	13.7328960539
C	-17.9648788685	-1.4569185894	14.8556907129
O	-19.2167519530	-1.2799798065	14.8862566122
O	-17.3496901120	-2.1619651801	15.7165424344
H	-18.4821882912	-1.4509470435	12.1139542299

H	-16.3257856859	-1.4505741071	13.4844594596
H	-16.7365296926	0.1178529630	14.1281659104
C	-21.9319999624	-3.3250000086	12.2140001575
C	-21.6188544658	-3.5839150896	13.6989794383
C	-22.3239831526	-2.5779009216	14.6288976144
C	-22.1213737203	-2.8474940400	16.1306010798
N	-20.7242171467	-2.6279549213	16.5297487305
C	-20.2780118588	-2.8540964160	17.7482050845
N	-21.0855658715	-3.1904850027	18.7737737288
N	-18.9320530469	-2.7647322929	18.0064942059
H	-21.5982261361	-2.3237262424	11.9151328638
H	-21.9227928704	-4.6061301178	13.9693379485
H	-20.5357712444	-3.5232856229	13.8577360787
H	-21.9732904969	-1.5632618426	14.3990350062
H	-23.4060442603	-2.5950998228	14.4334833548
H	-22.7820256429	-2.1811632104	16.7078856554
H	-22.4087202982	-3.8843741712	16.3621201783
H	-20.0624088290	-2.1105670260	15.8502360989
H	-22.0577772900	-3.3699274856	18.5812625744
H	-20.6635604865	-3.6910190938	19.5651043558
H	-18.3284024574	-2.4663473521	17.2126562295
H	-18.6882392513	-2.2689364461	18.8590764955
C	-16.2809998659	-5.8030000414	12.1999997757
C	-16.5354757924	-6.0945144697	13.6897311524
C	-17.2258830663	-4.8854095835	14.3690656852
C	-17.3060346391	-5.0116996742	15.8777445351
O	-18.2504077925	-5.6685313424	16.3840690032
O	-16.4143783138	-4.4698447212	16.6544161847
H	-15.6864698613	-4.8937953984	12.0742385239
H	-17.1627986216	-6.9896277657	13.7994379091
H	-15.5884511574	-6.3081959707	14.1967471015
H	-16.6732852026	-3.9844161175	14.1110882699
H	-18.2518143882	-4.7967004859	13.9901782132
C	-16.3929999554	-9.8490000265	16.0549999544
C	-16.6744481341	-9.0396343666	17.3297984135
C	-15.7520454224	-7.8297101549	17.5041820302
O	-14.6676012761	-7.7981112446	16.8761251456
O	-16.1250212470	-6.8973061492	18.3058992990
H	-16.5538242646	-9.2350959790	15.1623683466
H	-17.7135976112	-8.6856175046	17.3523469868
H	-16.5477090215	-9.6735623986	18.2212004448
C	-17.5420000402	-9.6659997373	21.8140000295
C	-17.0686594118	-8.2274270973	22.0683818979
C	-17.8299097655	-7.1116872640	21.3673561347

O	-19.0524085600	-7.2492233588	21.0727504636
O	-17.1934615648	-6.0200886391	21.1389067431
H	-18.6036993949	-9.7818660948	22.0565933792
H	-17.1446140872	-8.0026385510	23.1433087761
H	-16.0125228932	-8.1082143460	21.8165350656
C	-14.0159999882	-9.9710000386	25.1559999665
C	-14.5817131327	-8.8041578999	24.3648187841
C	-13.8689392509	-7.4708091894	24.6589032518
C	-14.3712519704	-6.4124072400	23.6981857672
O	-15.0188722203	-5.4123581146	24.1312470437
O	-14.1778305203	-6.6219219209	22.4526803658
H	-14.5420497114	-10.9070619183	24.9280699463
H	-14.4926789842	-9.0082038951	23.2927684678
H	-15.6524682601	-8.6976170776	24.5844030569
H	-14.0397328898	-7.1520610946	25.6929213136
H	-12.7906252895	-7.5869742517	24.5013810493
C	-10.0720000062	-10.4519999873	20.3670000095
C	-11.0767432336	-9.3327313138	20.6792335502
O	-11.2821608660	-8.4977614885	19.5121772027
C	-10.6612532716	-8.4906005107	21.8897985369
H	-10.3974056711	-11.0189503316	19.4884275184
H	-12.0587507924	-9.7872887529	20.8726774807
H	-10.5611067058	-7.8103892249	19.4434655334
H	-11.4125352163	-7.7284467812	22.1168963873
H	-10.5294644510	-9.1252888679	22.7757528488
H	-9.7149088040	-7.9783652445	21.6824500790
C	-9.3519999851	-7.6869999646	26.4129999415
C	-9.6488676906	-6.9246589492	25.1069277231
C	-9.9740967801	-5.4284182747	25.3154875267
C	-10.5724624155	-4.7756973615	24.0633766040
O	-11.4942677697	-5.3354625651	23.4542204484
N	-10.0786165916	-3.5752519138	23.7001692386
H	-8.4902631827	-7.2604684632	26.9431767131
H	-8.7952588708	-7.0157393378	24.4212990858
H	-10.5005051428	-7.3853827522	24.5976879410
H	-10.7320970495	-5.3340364708	26.1074843027
H	-9.0836518757	-4.8843232348	25.6594988675
H	-9.3023640751	-3.1707166946	24.1979656497
H	-10.4428419756	-3.0689157026	22.8819662931
P	-15.6743908474	-2.2565066626	19.4026629864
O	-16.1847566941	-3.6470042119	19.8743099791
O	-14.2152783037	-1.9892203349	19.7464261121
O	-16.2255331205	-1.8528576844	18.0291996106
O	-16.5495210527	-1.2570730298	20.4557486427

Ca	-13.8640498457	-5.6355577532	17.6796894822
Ca	-17.6588383072	-5.1515213072	18.7570941483
Ca	-15.3575220807	-4.6172283830	21.8597883885
Fe	-12.8189708857	-2.3346019877	18.2425622278
Fe	-15.4097456505	-2.6741506966	16.3759700033
O	-14.1383020214	-3.3175279978	17.4083387993
O	-12.3296293493	-4.1647011006	19.0284737125
O	-13.0725354162	-3.9486426141	21.6950328458
O	-16.5183906558	-2.6574180861	22.7504609826
O	-19.5407770859	-4.6013895889	20.6469507060
O	-19.7069843046	-6.5952032433	18.5258763221
O	-13.3951134122	-6.9245071916	19.7284509509
H	-7.0176071099	-7.1078368441	19.9770107328
H	-5.7878276891	-5.8933864968	20.4151759615
H	-7.6712685866	1.0314237636	21.8610300063
H	-6.7289425375	-0.3050604256	22.5489384487
H	-8.4472502357	-2.4811625225	16.2067775501
H	-8.2016690788	-0.8958491789	16.9719660354
H	-12.1653488388	3.6307743911	15.7305056797
H	-10.9259859410	2.9682305475	14.6478690620
H	-11.1819579183	-2.7621148147	12.0567984658
H	-12.3025703794	-1.4976191904	11.5089235509
H	-18.9054700550	0.1193677949	12.8000201339
H	-17.4964705939	-0.0301494854	11.7240157522
H	-21.4234736172	-4.0523745585	11.5712099374
H	-23.0098535121	-3.3949350112	12.0154697144
H	-15.7453042223	-6.6296350068	11.7168139109
H	-17.2278355799	-5.6586159616	11.6609051173
H	-15.3519549057	-10.1821302863	16.0392007863
H	-17.0480296862	-10.7270271131	15.9938434810
H	-17.4059017439	-9.9444843368	20.7622592110
H	-16.9646847536	-10.3684090878	22.4252847342
H	-12.9532945405	-10.1247957103	24.9262311051
H	-14.0960918109	-9.8022106381	26.2386450833
H	-9.0855714162	-10.0230049456	20.1521055129
H	-9.9748520347	-11.1405544657	21.2162375494
H	-10.2133264298	-7.6520527766	27.0924362422
H	-9.1295516170	-8.7399561345	26.2054883171
H	-19.6233010302	-7.2438717879	19.2506016198
H	-19.5021341833	-7.0158923603	17.6788780351
H	-19.0129560223	-4.2189100468	21.3615341022
H	-19.5349167751	-5.5811392223	20.8442560820
H	-16.5758446459	-2.0064021403	22.0047154999
H	-16.1346621962	-2.1992370999	23.5074747738

H	-12.5482767194	-3.1003569878	21.5676049689
H	-12.4831171380	-4.5246853267	22.2411888422
H	-11.2744444725	-4.3278167853	19.1102601082
H	-12.6234190997	-4.1781969361	19.9691233299
H	-12.6089993992	-7.5354887550	19.6574883366
H	-13.6082716851	-6.9014212730	20.6767884316
C	-16.2540452115	0.1480107229	20.3734780522
H	-16.8482598050	0.6505825766	21.1421424992
H	-15.1870182222	0.3238483680	20.5425172220
H	-16.5336714822	0.5303008823	19.3868669194

Enzyme-methyl phosphate complex indicated in entry 5 of Table S1

Energy with the medium-sized basis set:	-5503.03959
Solution energy with the medium-sized basis set:	-5503.12101
Energy with larger basis sets:	-5505.08030
Zero-point energy:	1.60986
Dispersion effect:	-0.33829

C	-6.8650001660	-6.1059999243	20.3889999297
C	-7.6487422946	-5.0372133580	19.6226010104
C	-9.1458538589	-5.3703814764	19.4595927439
O	-9.4833898834	-6.5721278112	19.5633795360
O	-9.8885710931	-4.3665009281	19.2088200776
H	-7.2316367868	-6.1976691751	21.4189316201
H	-7.5660165619	-4.0553731329	20.1054787388
H	-7.2310017753	-4.9140180238	18.6112312481
C	-7.4140000029	-0.0289999893	21.7370000094
C	-8.7042547293	-0.8659623928	21.7907626153
C	-9.6137156582	-0.6151926907	20.5801769843
C	-10.9117518108	-1.4309265589	20.5384564981
O	-11.2775353524	-2.0609748335	21.5626352217
O	-11.5358433681	-1.3469116539	19.4296992127
H	-6.8341541742	-0.2598443608	20.8344710608
H	-8.4470758054	-1.9333946475	21.8257860253
H	-9.2579268237	-0.6431253688	22.7129666870
H	-9.8995202504	0.4472224590	20.5340550207
H	-9.0711144059	-0.8220955945	19.6502870571
C	-8.8830000729	-1.7599999602	16.9099999715
C	-10.2114220152	-1.0817034101	16.5702840616
S	-11.4845493586	-2.3555223690	16.2820224462
H	-9.0003357914	-2.4363498665	17.7629077706
H	-10.5539818982	-0.4816855804	17.4177709361
H	-10.1148198156	-0.4423168459	15.6876888838

C	-11.9689999749	2.8629998529	14.9700001023
C	-12.3474168452	1.5079612826	15.5766041634
C	-13.7529442486	1.4688600256	16.2178587822
C	-14.0816460452	0.0455597499	16.6844543154
O	-13.3052828495	-0.3963159685	17.6006879214
O	-15.0222341329	-0.5550247051	16.1145282598
H	-12.6655818671	3.1534549903	14.1723178733
H	-12.2925668400	0.7326842644	14.7996880101
H	-11.6182175835	1.2347947919	16.3440826759
H	-13.7827470316	2.1497459428	17.0797977333
H	-14.5176905110	1.7859235373	15.5002589078
C	-12.1639999448	-2.3060000175	12.2389999896
C	-13.1700018646	-3.4609776720	12.1043447392
C	-13.0570944437	-4.5056064086	13.2298315652
C	-13.8194427458	-4.2280557856	14.5427636055
O	-14.6526555413	-3.2599789476	14.5609085776
O	-13.5751152600	-5.0299968163	15.4825700205
H	-12.2979445906	-1.7939346823	13.1980858687
H	-14.1882739078	-3.0542726487	12.1015692412
H	-13.0187092945	-3.9576763030	11.1338895369
H	-13.4196749964	-5.4820283044	12.8787629749
H	-12.0059360236	-4.6677994536	13.5033435225
C	-18.0649999783	-0.5230000985	12.5230001702
C	-17.3216069894	-0.9609010078	13.7787615878
C	-18.2288071523	-1.5924844071	14.8187209116
O	-19.4774647086	-1.4799883286	14.7246157366
O	-17.6615855430	-2.2267285248	15.7775960077
H	-18.5341783926	-1.3780476123	12.0222764238
H	-16.5159717047	-1.6697210776	13.5489114515
H	-16.8148842806	-0.1156230737	14.2645088186
C	-21.9319999676	-3.3250000104	12.2140001481
C	-21.8353014453	-3.7203421286	13.6956689061
C	-22.5609536302	-2.7154262018	14.6102760367
C	-22.3836707539	-2.9970889927	16.1117186080
N	-20.9857579927	-2.7820966399	16.5098817185
C	-20.5242074165	-3.0248914823	17.7226488450
N	-21.3232775362	-3.3676387101	18.7509350019
N	-19.1775223136	-2.9486284528	17.9572414178
H	-21.4433403065	-2.3583021266	12.0439944901
H	-22.2586353499	-4.7243234771	13.8480739474
H	-20.7785235414	-3.7752066995	13.9809818105
H	-22.1947419235	-1.7029229329	14.3966048411
H	-23.6372067900	-2.7215285828	14.3867717105
H	-23.0443336871	-2.3326027091	16.6903830306

H	-22.6725778310	-4.0351357916	16.3352688199
H	-20.3396428792	-2.2928645062	15.8166313871
H	-22.2987792566	-3.5429760065	18.5723643263
H	-20.8837638593	-3.8595196979	19.5382426417
H	-18.5983277102	-2.6328376459	17.1465579531
H	-18.8972552352	-2.4539993515	18.7988809561
C	-16.2809998736	-5.8030000348	12.1999997882
C	-16.5296223800	-6.1766256951	13.6717501962
C	-17.3221568202	-5.0517901105	14.3789611577
C	-17.4233833248	-5.2197049535	15.8826445389
O	-18.3835815444	-5.8680711408	16.3739864503
O	-16.5362019694	-4.6740557396	16.6529437645
H	-15.7274425493	-4.8620933246	12.1287590769
H	-17.0837820898	-7.1228441469	13.7374949856
H	-15.5764762029	-6.3314871013	14.1889702744
H	-16.8185057028	-4.1087584613	14.1653947119
H	-18.3404591808	-5.0148230632	13.9721760680
C	-16.3929999599	-9.8490000474	16.0549999403
C	-16.5869241036	-9.3062134330	17.4749319991
C	-15.9519363374	-7.9282599638	17.6800357322
O	-14.9658548862	-7.6101397929	16.9719326440
O	-16.4554143801	-7.1752801920	18.5829836580
H	-16.8694728460	-9.1918358090	15.3188849063
H	-17.6510403963	-9.2431472489	17.7373957634
H	-16.1288435580	-9.9881101289	18.2082196015
C	-17.5420000448	-9.6659997593	21.8140000374
C	-17.1183025616	-8.2176283086	22.1121211743
C	-17.9314021178	-7.0897542441	21.4866173571
O	-19.1307994905	-7.2708476849	21.1284241168
O	-17.3595135313	-5.9441855474	21.3835371696
H	-18.5904429113	-9.8362337869	22.0819972161
H	-17.1603484176	-8.0381928378	23.1971073091
H	-16.0768220331	-8.0529071906	21.8247396868
C	-14.0160000105	-9.9710000578	25.1559999712
C	-14.6121160966	-8.7992348672	24.3987996209
C	-13.8105769545	-7.4992738659	24.6010931728
C	-14.3815351726	-6.4367685000	23.6921124904
O	-15.1039543002	-5.5111838446	24.1877192362
O	-14.1991236914	-6.5648922312	22.4419408047
H	-14.5983741826	-10.8891727964	25.0062030683
H	-14.6363290966	-9.0268198622	23.3279131314
H	-15.6501742254	-8.6382532710	24.7182877753
H	-13.8586956066	-7.1713625251	25.6449093416
H	-12.7639542449	-7.6676559413	24.3296004978

C	-10.0720000096	-10.4519999950	20.3670000123
C	-11.1248023484	-9.3731243466	20.6765595537
O	-11.3204442191	-8.5100707565	19.5299444137
C	-10.7759795486	-8.5539052890	21.9254482502
H	-10.3508900167	-11.0030409242	19.4628163895
H	-12.0963558442	-9.8652278113	20.8243595230
H	-10.6225639426	-7.8028805822	19.5195350196
H	-11.5568792018	-7.8163563725	22.1366405380
H	-10.6640636956	-9.2073901185	22.8008921668
H	-9.8367737656	-8.0121854714	21.7673430557
C	-9.3519999940	-7.6869999685	26.4129999398
C	-9.6726541961	-6.8966025860	25.1324936238
C	-9.9170521627	-5.3913444263	25.3811531236
C	-10.5643070353	-4.7043980334	24.1766857301
O	-11.5612966001	-5.2092099132	23.6430400245
N	-10.0279775108	-3.5368181105	23.7675980690
H	-8.4489878453	-7.3064790432	26.9083951231
H	-8.8579673757	-7.0154360356	24.4053574951
H	-10.5688436309	-7.3086991415	24.6594774418
H	-10.6188617625	-5.2776834447	26.2207100353
H	-8.9842080229	-4.8905882815	25.6741692126
H	-9.1871694463	-3.1835118544	24.1945747202
H	-10.4131859938	-3.0251155744	22.9644921697
P	-15.7770164447	-2.6601271650	19.5193627244
O	-15.7511018055	-4.2314269661	19.5311743553
O	-14.4548025233	-2.0258748163	19.9347215923
O	-16.5880685595	-2.0835013557	18.3745483483
O	-16.7378529147	-2.5230083379	20.9311528560
Ca	-14.2227716637	-5.4359856420	17.7881978606
Ca	-17.8133478237	-5.2819275889	18.7557061215
Ca	-15.4562860204	-4.5738919730	21.8927486117
Fe	-12.9604457766	-2.2321512764	18.3864339693
Fe	-15.6730711958	-2.5706142527	16.3416051352
O	-14.0863060520	-3.0504718061	17.4302996221
O	-12.3772692410	-4.1452449590	19.1005421373
O	-13.1147824797	-3.9249188128	21.8194083513
O	-15.2220658505	-2.8708815444	23.7951183949
O	-19.6646774800	-4.7066288715	20.5696365417
O	-19.8166470142	-6.8064668519	18.5264901774
O	-13.4793590995	-6.9007354280	19.6596515830
H	-6.9949024741	-7.0818393180	19.9125009483
H	-5.7933578460	-5.8695281370	20.4293978431
H	-7.6398636136	1.0452963499	21.7204776206
H	-6.7719909783	-0.2228910183	22.6055226385

H	-8.5086864147	-2.3503523771	16.0646418317
H	-8.1209944512	-1.0043242868	17.1492814082
H	-11.9852214455	3.6573133120	15.7287078901
H	-10.9606888157	2.8341671721	14.5380882231
H	-11.1312311910	-2.6784984508	12.2012266475
H	-12.2873230596	-1.5697287720	11.4334784233
H	-18.8608106604	0.1889517237	12.7649861769
H	-17.3807292435	-0.0474672597	11.8095980491
H	-21.4399619387	-4.0661334396	11.5737613851
H	-22.9775925125	-3.2401765256	11.8878205432
H	-15.7031615110	-6.5783698506	11.6814540202
H	-17.2302168684	-5.6765699022	11.6608113811
H	-15.3284513652	-9.8949203935	15.8108480744
H	-16.8251063471	-10.8524361068	15.9498575585
H	-17.4253435198	-9.8924909430	20.7483955263
H	-16.9180682694	-10.3658576501	22.3810153378
H	-12.9893529353	-10.1735121947	24.8237322729
H	-13.9790198022	-9.7759286037	26.2364240355
H	-9.0940662927	-9.9851317096	20.1969816564
H	-9.9798524142	-11.1611233064	21.1997497343
H	-10.1793690323	-7.6227019817	27.1313582278
H	-9.1866542908	-8.7461743673	26.1852144823
H	-19.6700298233	-7.4487255757	19.2444698824
H	-19.5324910998	-7.1932239688	17.6847706977
H	-19.1251176687	-4.3111758137	21.2693181438
H	-19.6575287818	-5.6825949686	20.8120827712
H	-14.3607505242	-2.4855252218	23.5788781591
H	-15.0207421606	-3.6610395769	24.3387558546
H	-12.5974726271	-3.0914815997	21.6488028096
H	-12.5194015737	-4.4811028938	22.3775137738
H	-11.3365500435	-4.3142449439	19.0874066527
H	-12.6311151601	-4.2225558940	20.0456354898
H	-12.7046807047	-7.5144949262	19.5800284751
H	-13.6863457168	-6.8856021167	20.6079669313
C	-16.9142101066	-1.2034558575	21.4702918500
H	-17.4112479809	-1.3051508237	22.4377371993
H	-15.9456912750	-0.7131025701	21.6060380153
H	-17.5312509603	-0.5988010368	20.7952837027

Enzyme-methyl phosphate complex indicated in entry 6 of Table S1

Energy with the medium-sized basis set:	-5503.07275
Solution energy with the medium-sized basis set:	-5503.15732
Energy with larger basis sets:	-5505.13221

Zero-point energy:	1.60951
Dispersion effect:	-0.33592

C	-6.8650001645	-6.1059999085	20.3889999152
C	-7.5979421154	-5.0905030601	19.5093584764
C	-9.0985771441	-5.4042912938	19.3666085370
O	-9.4303703911	-6.6145583177	19.3461704828
O	-9.8515556356	-4.3854566413	19.2592915221
H	-7.2460710436	-6.0815651856	21.4180878280
H	-7.4902392840	-4.0711077353	19.8966766776
H	-7.1640029395	-5.0903430982	18.4973967420
C	-7.4140000720	-0.0290000201	21.7369999787
C	-8.7429516847	-0.7847667131	21.9139118849
C	-9.5894112051	-0.7449188100	20.6366260476
C	-10.9481974042	-1.4470453413	20.6842489099
O	-11.3135048910	-2.0543951483	21.7235898544
O	-11.6277760648	-1.3272480003	19.6139504524
H	-6.8243904281	-0.4619599131	20.9190310440
H	-8.5399053877	-1.8308683468	22.1787451050
H	-9.3131455844	-0.3535186001	22.7485982644
H	-9.7748447351	0.2961443389	20.3340537393
H	-9.0361253847	-1.2043517058	19.8069009835
C	-8.8830000535	-1.7600000150	16.9099999912
C	-10.2342737922	-1.0724693631	16.7380197525
S	-11.5614392990	-2.3170703768	16.4495238095
H	-8.9218464931	-2.4836117583	17.7309299227
H	-10.4925072777	-0.4964564518	17.6295723485
H	-10.2125459989	-0.3960197764	15.8766621946
C	-11.9689999991	2.8629999017	14.9700000869
C	-12.3605527766	1.5219157567	15.6120673608
C	-13.8533481517	1.4117907657	16.0096720786
C	-14.1448804191	0.0305545057	16.6072170064
O	-13.6036514936	-0.2448449808	17.7087395621
O	-14.8813825945	-0.7453543723	15.9111742086
H	-12.5346070635	3.0444577621	14.0464467251
H	-12.1233856815	0.7040699323	14.9187235837
H	-11.7581942666	1.3531162870	16.5107727085
H	-14.0878079783	2.1770413410	16.7625574383
H	-14.4969099453	1.5742901496	15.1380696399
C	-12.1639999454	-2.3060000152	12.2389999859
C	-13.2542330195	-3.3786299438	12.1018650895
C	-13.1294355520	-4.4838643895	13.1635150294
C	-13.8179501698	-4.2638518534	14.5198550902
O	-14.6801549225	-3.3150695406	14.6202016759

O	-13.5155370553	-5.0915826451	15.4097575943
H	-12.1970738127	-1.8514250961	13.2357328115
H	-14.2425122318	-2.9109528806	12.1857637944
H	-13.1955646376	-3.8292768541	11.0998726447
H	-13.5347569199	-5.4314423428	12.7833766987
H	-12.0743445398	-4.6872700240	13.3864909179
C	-18.0649999790	-0.5230001105	12.5230001713
C	-17.2741864481	-0.7426791005	13.8074784601
C	-18.1273496430	-1.3798482948	14.8898302002
O	-19.3726504541	-1.1767133220	14.8865640436
O	-17.5477825573	-2.1077403946	15.7615922921
H	-18.4120421732	-1.4761304709	12.1052130584
H	-16.3888963702	-1.3651321023	13.6434618041
H	-16.8932875270	0.2087426875	14.2032903547
C	-21.9319999660	-3.3250000078	12.2140001508
C	-21.7055886732	-3.5819840145	13.7135850514
C	-22.4386077594	-2.5566455232	14.5988670243
C	-22.2771550296	-2.8009259691	16.1091463833
N	-20.8879818061	-2.5799418449	16.5322792134
C	-20.4448800625	-2.8554166494	17.7439755155
N	-21.2550307015	-3.2411233811	18.7491868529
N	-19.1044396821	-2.7695572516	18.0117723049
H	-21.5532638099	-2.3360399054	11.9284988781
H	-22.0437742801	-4.5962406975	13.9731904869
H	-20.6316445110	-3.5430441500	13.9301495271
H	-22.0775188107	-1.5475137492	14.3612138404
H	-23.5140289633	-2.5753249814	14.3703617368
H	-22.9490713505	-2.1250206206	16.6615007973
H	-22.5709349860	-3.8338851817	16.3492927691
H	-20.2335002462	-2.0422287013	15.8729853038
H	-22.2291693212	-3.4045477019	18.5535643057
H	-20.8304724869	-3.7605494832	19.5265350032
H	-18.5003265731	-2.4409460154	17.2294419501
H	-18.8628411330	-2.3105003616	18.8849513767
C	-16.2809998664	-5.8030000378	12.1999997722
C	-16.5851609179	-6.0830903182	13.6815149248
C	-17.4112397214	-4.9289024483	14.3018753422
C	-17.5334023818	-5.0354057187	15.8098046604
O	-18.4898480412	-5.6723306979	16.3187870018
O	-16.6376108556	-4.4884324013	16.5678241632
H	-15.7518699972	-4.8526581667	12.0844726190
H	-17.1372520571	-7.0277106322	13.7827002458
H	-15.6508362222	-6.2050037309	14.2399433815
H	-16.9217230794	-3.9863193243	14.0533735775

H	-18.4213316943	-4.9326335636	13.8743615647
C	-16.3929999554	-9.8490000302	16.0549999508
C	-16.6866430166	-8.9998147659	17.3008551480
C	-15.7800776859	-7.7738301564	17.4448956959
O	-14.6988901361	-7.7358945311	16.8112040965
O	-16.1601024779	-6.8348886788	18.2363601537
H	-16.5623831763	-9.2694243611	15.1411629757
H	-17.7300190181	-8.6577511385	17.3088087911
H	-16.5558989021	-9.6025243510	18.2130303847
C	-17.5420000367	-9.6659997087	21.8140000242
C	-17.1593058741	-8.2132827845	22.1274125399
C	-17.9249157759	-7.1343487618	21.3751466181
O	-19.1457027175	-7.3001017294	21.0865194552
O	-17.2970290028	-6.0505343598	21.0998091836
H	-18.6115593535	-9.8360793526	21.9770536185
H	-17.3315574743	-8.0127309950	23.1964974748
H	-16.0955975557	-8.0419973561	21.9530653411
C	-14.0159999838	-9.9710000279	25.1559999563
C	-14.5833611810	-8.8337238060	24.3220682745
C	-13.9042030211	-7.4813090189	24.6087435427
C	-14.4445687943	-6.4323436583	23.6580884179
O	-15.1229083725	-5.4595458606	24.1029852467
O	-14.2471548749	-6.6194965825	22.4087833663
H	-14.5184239828	-10.9223253159	24.9380061082
H	-14.4638939067	-9.0590416491	23.2567626820
H	-15.6609327856	-8.7441454107	24.5120087323
H	-14.0763658609	-7.1691200173	25.6446779613
H	-12.8242236878	-7.5674983282	24.4436802962
C	-10.0720000022	-10.4519999947	20.3670000127
C	-11.0838964325	-9.3397529445	20.6843526367
O	-11.2918455608	-8.4981431459	19.5223184362
C	-10.6765401482	-8.5013765652	21.9010692420
H	-10.3930484966	-11.0147824204	19.4842368611
H	-12.0637356533	-9.8010106285	20.8723145931
H	-10.5778608619	-7.8053800471	19.4661675200
H	-11.4323766732	-7.7423101979	22.1255002351
H	-10.5486147737	-9.1391728927	22.7854940901
H	-9.7306264949	-7.9855372380	21.7009593219
C	-9.3519999761	-7.6870000353	26.4130000137
C	-9.6674700513	-6.8654138437	25.1511366068
C	-10.1319024339	-5.4247950269	25.4575426764
C	-10.6958529474	-4.7232272566	24.2198100832
O	-11.5590980354	-5.2854553309	23.5315763011
N	-10.2291842667	-3.4885833561	23.9488393577

H	-8.5516172161	-7.2249578107	27.0059834089
H	-8.7842974805	-6.8295792963	24.4984476301
H	-10.4553106947	-7.3588277014	24.5739813794
H	-10.9447324083	-5.4607896541	26.1975827764
H	-9.3138903855	-4.8449438420	25.9069114593
H	-9.5093947524	-3.0807753104	24.5229706993
H	-10.5598880435	-2.9585453608	23.1304175388
P	-15.9452716217	-2.2088628550	19.5272799571
O	-16.4347590673	-3.6292090491	19.9285764686
O	-14.4979509225	-1.9504866097	19.9250201854
O	-16.4578603750	-1.7736192889	18.1547816719
O	-16.8685270668	-1.2753349069	20.6067726098
Ca	-13.8891750434	-5.6046625672	17.6965063854
Ca	-17.7871332330	-5.1697987281	18.7067284938
Ca	-15.4755938679	-4.6204422565	21.8441228499
Fe	-12.9599781532	-2.1958203043	18.3831945146
Fe	-15.5320647279	-2.6108224526	16.3915338181
O	-14.3068099753	-3.3015951645	17.5284070721
O	-12.3342398362	-4.2296108800	19.1238735286
O	-13.1652283325	-3.9585095377	21.7697600255
O	-16.6582055831	-2.7334161030	22.8509996489
O	-19.6737874542	-4.6607471007	20.5946848339
O	-19.7700626075	-6.6929745484	18.5321737676
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