

Supplementary material

An *ab initio* parameterized interatomic force field for hydroxyapatite.

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Ulderico Segre^a and Piero Ugliengo^{*b}

5

1) GULP input of the optimization and phonon calculation for hexagonal P6₃ HA

```
#
# Keywords:
#
10 opti conp compare phon angle nono
#
# Options:
#
title
15 hexagonal HA - optimization
end
name HA
cell
  9.328617  9.328617  6.949405  90.000000  90.000000 120.000000
20 fractional
Ca1 core 1/3      2/3      0.9975439 2.0000000 1.00000 0.00000
Ca1 core 2/3      1/3      0.0002482 2.0000000 1.00000 0.00000
Ca2 core 0.2443840 0.9899708 0.2492715 2.0000000 1.00000 0.00000
P1 core 0.3942981 0.3658030 0.2505560 5.0000000 1.00000 0.00000
25 O1 core 0.3178804 0.4802150 0.2531038 1.5609290 1.00000 0.00000
O1 core 0.5864274 0.4658338 0.2430649 1.5609290 1.00000 0.00000
O1 core 0.3326459 0.2498868 0.0736627 1.5609290 1.00000 0.00000
O1 core 0.6517670 0.7433956 0.9324463 1.5609290 1.00000 0.00000
O2 core 0.0000000 0.0000000 0.7906321 0.4941546 1.00000 0.00000
30 H1 core 0.0000000 0.0000000 0.9302591 1.0000000 1.00000 0.00000
O1 shel 0.3178804 0.4802150 0.2531038 -3.5609290 1.00000 0.00000
O1 shel 0.5864274 0.4658338 0.2430649 -3.5609290 1.00000 0.00000
O1 shel 0.3326459 0.2498868 0.0736627 -3.5609290 1.00000 0.00000
O1 shel 0.6517670 0.7433956 0.9324463 -3.5609290 1.00000 0.00000
35 O2 shel 0.0000000 0.0000000 0.7906321 -2.4941546 1.00000 0.00000
space
173
species 7
P core 5.000000
40 Ca core 2.000000
H core 1.000000
O1 core 1.560929
O1 shel -3.560929
O2 core 0.494155
45 O2 shel -2.494155
spring
O1 145.770418 0
spring
O2 43.887532 0
50 buck
P1 core O1 shel 1099.278765 0.342928 0.0000000 0.00 15.00 0 0 0
buck
Ca1 core O1 shel 3074.425319 0.288162 0.0000000 0.00 15.00 0 0 0
buck
55 Ca2 core O1 shel 2899.545766 0.288626 0.0000000 0.00 15.00 0 0 0
buck
Ca2 core O2 shel 948.04598 0.344000 0.0000000 0.00 15.00 0 0 0
buck
H1 core O2 shel 463.27569 0.205814 0.0000000 0.00 15.00 0 0 0
60 buck
O1 shel O1 shel 122152.69 0.15291 35.8699 0.00 15.00 0 0 0
buck
O1 shel O2 shel 846.47487 0.213327 0.090075 0.00 15.00 0 0 0
buck
65 O2 shel O2 shel 54718.655 0.253276 62.6727 0.00 15.00 0 0 0
```

70

75

2) CRYSTAL06 input for the frequency calculation of hexagonal P6₃ HA and list of all the computed frequencies

```
HAP
CRYSTAL
80 0 0 0
173
9.32861726 6.94940471
10
220 3.333333333333333E-01 -3.333333333333333E-01 -2.456023551711E-03
85 220 -3.333333333333333E-01 3.333333333333333E-01 2.482241275054E-04
220 2.443840782128E-01 -1.002912506776E-02 2.492715740572E-01
15 3.942981565720E-01 3.658030983991E-01 2.505560288223E-01
8 3.178804981007E-01 4.802150573665E-01 2.531038069180E-01
8 -4.135725529085E-01 4.658338011070E-01 2.430649979592E-01
90 8 3.326459275406E-01 2.498868133568E-01 7.366270117730E-02
8 -3.482329741991E-01 -2.566043560930E-01 -6.755362047962E-02
8 0.000000000000E+00 0.000000000000E+00 -2.093678348920E-01
1 0.000000000000E+00 0.000000000000E+00 -6.974083104290E-02
FREQCALC
95 INTENS
END
END
220 2
HAYWSC
100 0 1 3 8. 1.
5.3568 -1.4687 -0.0794
1.71 -1.8752 0.2902
1.0 3.4301 0.1427
0 1 1 2. 1.
105 0.500 1.0 1.0
8 4
0 0 6 2. 1.
5484.6717 0.0018
825.2349 0.0140
110 188.0470 0.0684
52.9645 0.2327
16.8976 0.4702
5.7996 0.3585
0 1 3 6. 1.
115 15.5396 -0.1108 0.0709
3.5999 -0.1480 0.3398
1.0138 1.1308 0.7272
0 1 1 0. 1.
0.2742 1. 1.
120 0 3 1 0. 1.
0.538 1.
15 5
0 0 8 2. 1.
202703. 0.0001
125 22413.1 0.0013
4625.08 0.0068
1312.41 0.0275
425.149 0.0951
146.409 0.2667
130 51.8363 0.4781
18.5913 0.2971
0 1 5 8. 1.
339.375 0.00089 0.00287
94.9248 -0.03549 0.02778
135 23.125 -0.153 0.172
6.9753 0.355 0.4215
2.275 0.9102 0.4109
0 1 2 5. 1.
```

140 1.219 -0.3715 0.09158
 0.48105 1.271 0.9349
 0 1 1 0. 1.
 0.135 1. 1.
 0 3 1 0. 1.
 0.74583 1.

145 1 3
 0 0 3 1. 1.00
 0.1873113696D+02 0.3349460434D-01
 0.2825394365D+01 0.2347269535D+00
 0.6401216923D+00 0.8137573262D+00

150 0 0 1 0. 1.00
 0.1612777588D+00 0.1000000000D+01
 0 2 1 0. 1.
 1.1 1.

99 0
 155 END
 DFT
 B3LYP
 XLGRID
 END

160 TOLINTEG
 6 6 6 6 14
 SHRINK
 4 4
 LEVSHIFT

165 6 1
 FMIXING
 30
 END

170

175

3) CRYSTAL06 output harmonic frequencies for HA

	MODES	EIGV (HARTREE**2)	FREQUENCIES (CM**-1)	IRREP	IR	INTENS (KM/MOL)	RAMAN
180	1- 2	-0.6891E-08	-18.2186	-0.5462	(E1)	A (86.15)	A
	3- 3	-0.2252E-10	-1.0415	-0.0312	(A)	A (0.00)	A
	4- 5	0.3643E-10	1.3246	0.0397	(E1)	A (0.76)	A
185	6- 6	0.1497E-06	84.9096	2.5455	(B)	I (0.00)	I
	7- 8	0.2313E-06	105.5502	3.1643	(E2)	I (0.00)	A
	9- 9	0.2795E-06	116.0237	3.4783	(A)	A (43.90)	A
	10- 11	0.3184E-06	123.8504	3.7129	(E1)	A (324.07)	A
	12- 13	0.4147E-06	141.3323	4.2370	(E2)	I (0.00)	A
190	14- 15	0.5544E-06	163.4160	4.8991	(E1)	A (15.76)	A
	16- 17	0.5762E-06	166.5981	4.9945	(E2)	I (0.00)	A
	18- 19	0.6097E-06	171.3765	5.1377	(E2)	I (0.00)	A
	20- 20	0.6746E-06	180.2670	5.4043	(B)	I (0.00)	I
	21- 21	0.7320E-06	187.7716	5.6293	(A)	A (0.27)	A
195	22- 22	0.7596E-06	191.2886	5.7347	(B)	I (0.00)	I
	23- 23	0.8611E-06	203.6653	6.1057	(A)	A (21.28)	A
	24- 25	0.9355E-06	212.2772	6.3639	(E2)	I (0.00)	A
	26- 26	0.9721E-06	216.3921	6.4873	(B)	I (0.00)	I
200	27- 28	0.1004E-05	219.9102	6.5927	(E1)	A (176.33)	A
	29- 29	0.1076E-05	227.6210	6.8239	(A)	A (10.13)	A
	30- 30	0.1117E-05	231.9479	6.9536	(B)	I (0.00)	I
	31- 31	0.1186E-05	239.0424	7.1663	(A)	A (93.77)	A
	32- 33	0.1253E-05	245.6269	7.3637	(E1)	A (1335.36)	A
	34- 35	0.1279E-05	248.1678	7.4399	(E2)	I (0.00)	A
205	36- 37	0.1326E-05	252.7537	7.5774	(E1)	A (734.38)	A
	38- 38	0.1366E-05	256.5527	7.6913	(A)	A (0.06)	A
	39- 39	0.1366E-05	256.5550	7.6913	(B)	I (0.00)	I
	40- 41	0.1453E-05	264.5150	7.9300	(E2)	I (0.00)	A
	42- 42	0.1582E-05	276.0804	8.2767	(B)	I (0.00)	I
	43- 44	0.1602E-05	277.7539	8.3269	(E2)	I (0.00)	A
210	45- 46	0.1605E-05	278.0478	8.3357	(E1)	A (161.80)	A
	47- 47	0.1754E-05	290.6813	8.7144	(B)	I (0.00)	I
	48- 49	0.1764E-05	291.4758	8.7382	(E1)	A (149.91)	A

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	50-	50	0.1840E-05	297.7122	8.9252	(A)	A (7.31)	A
215	51-	52	0.1864E-05	299.6079	8.9820	(E2)	I (0.00)	A
	53-	53	0.2127E-05	320.1216	9.5970	(A)	A (98.15)	A
	54-	54	0.2140E-05	321.0777	9.6257	(B)	I (0.00)	I
	55-	56	0.2224E-05	327.3309	9.8131	(E2)	I (0.00)	A
	57-	57	0.2277E-05	331.1478	9.9276	(B)	I (0.00)	I
220	58-	58	0.2298E-05	332.7251	9.9748	(A)	A (712.28)	A
	59-	60	0.2403E-05	340.2444	10.2003	(E1)	A (724.74)	A
	61-	62	0.2647E-05	357.0686	10.7046	(E2)	I (0.00)	A
	63-	63	0.2738E-05	363.1366	10.8866	(A)	A (322.89)	A
	64-	64	0.2765E-05	364.9325	10.9404	(B)	I (0.00)	I
225	65-	66	0.2976E-05	378.6346	11.3512	(E1)	A (4.85)	A
	67-	67	0.2993E-05	379.7077	11.3833	(B)	I (0.00)	I
	68-	68	0.3032E-05	382.1348	11.4561	(A)	A (166.73)	A
	69-	70	0.4236E-05	451.7217	13.5423	(E2)	I (0.00)	A
	71-	72	0.4375E-05	459.0882	13.7631	(E1)	A (680.39)	A
230	73-	74	0.4704E-05	476.0044	14.2703	(E1)	A (63.36)	A
	75-	75	0.4720E-05	476.8136	14.2945	(B)	I (0.00)	I
	76-	77	0.4821E-05	481.8769	14.4463	(E2)	I (0.00)	A
	78-	79	0.5185E-05	499.7769	14.9829	(E2)	I (0.00)	A
	80-	80	0.5322E-05	506.3356	15.1796	(A)	A (0.30)	A
235	81-	82	0.5500E-05	514.6947	15.4302	(E1)	A (118.44)	A
	83-	83	0.5770E-05	527.2145	15.8055	(A)	A (6.52)	A
	84-	84	0.5889E-05	532.5949	15.9668	(B)	I (0.00)	I
	85-	86	0.7262E-05	591.4310	17.7307	(E2)	I (0.00)	A
	87-	87	0.7440E-05	598.6576	17.9473	(A)	A (1037.58)	A
240	88-	89	0.7525E-05	602.0561	18.0492	(E1)	A (537.95)	A
	90-	90	0.7913E-05	617.4028	18.5093	(B)	I (0.00)	I
	91-	92	0.8018E-05	621.4682	18.6311	(E2)	I (0.00)	A
	93-	93	0.8245E-05	630.2146	18.8934	(A)	A (0.13)	A
	94-	95	0.8279E-05	631.4860	18.9315	(E1)	A (416.12)	A
245	96-	97	0.8474E-05	638.8898	19.1534	(E1)	A (424.90)	A
	98-	98	0.8665E-05	646.0396	19.3678	(B)	I (0.00)	I
	99-	99	0.8934E-05	656.0048	19.6665	(A)	A (6.92)	A
	100-	101	0.9138E-05	663.4556	19.8899	(E2)	I (0.00)	A
	102-	102	0.9182E-05	665.0353	19.9373	(B)	I (0.00)	I
250	103-	104	0.9645E-05	681.6241	20.4346	(E1)	A (1131.78)	A
	105-	106	0.1193E-04	758.2114	22.7306	(E2)	I (0.00)	A
	107-	108	0.2036E-04	990.2697	29.6875	(E1)	A (348.27)	A
	109-	109	0.2040E-04	991.3654	29.7204	(A)	A (6.00)	A
	110-	110	0.2041E-04	991.4459	29.7228	(B)	I (0.00)	I
255	111-	112	0.2046E-04	992.6623	29.7593	(E2)	I (0.00)	A
	113-	114	0.2420E-04	1079.6719	32.3677	(E1)	A (6409.39)	A
	115-	116	0.2423E-04	1080.4482	32.3910	(E2)	I (0.00)	A
	117-	117	0.2456E-04	1087.7424	32.6097	(A)	A (3934.05)	A
	118-	118	0.2514E-04	1100.3527	32.9877	(B)	I (0.00)	I
260	119-	120	0.2544E-04	1106.9987	33.1870	(E1)	A (155.63)	A
	121-	122	0.2553E-04	1108.8778	33.2433	(E2)	I (0.00)	A
	123-	123	0.2562E-04	1110.8551	33.3026	(A)	A (12.06)	A
	124-	125	0.2634E-04	1126.3146	33.7661	(E2)	I (0.00)	A
	126-	126	0.2636E-04	1126.7719	33.7798	(A)	A (11.26)	A
265	127-	128	0.2725E-04	1145.6851	34.3468	(E1)	A (427.91)	A
	129-	129	0.2753E-04	1151.6122	34.5245	(B)	I (0.00)	I
	130-	130	0.2888E-04	1179.5148	35.3610	(B)	I (0.00)	I
	131-	131	0.2954E-03	3772.2259	113.0885	(B)	I (0.00)	I
	132-	132	0.2958E-03	3774.4061	113.1538	(A)	A (38.23)	A

270 4) CRYSTAL06 input for the optimization of α -tricalciumphosphate (B3LYP)

```

ALFA TRICALCIUMPHOSPHATE
CRYSTAL
1 0 0
275 P 1 21/A
12.72673300000 27.52860200000 15.30374400000 126.858908
78
220 0.389320000000 0.027540000000 0.082380000000
220 0.155700000000 0.046000000000 0.331750000000
280 220 0.103940000000 0.074890000000 0.056080000000
220 0.121520000000 0.094360000000 0.552830000000
220 0.111070000000 0.080550000000 0.799980000000
220 0.356570000000 0.140450000000 0.318130000000
220 0.110680000000 0.194210000000 0.917620000000
    
```

285	220	0.344300000000	0.212660000000	0.668250000000
	220	0.396060000000	0.241560000000	0.943920000000
	220	0.378480000000	0.261030000000	0.447170000000
	220	0.388930000000	0.247220000000	0.200020000000
290	220	0.143430000000	0.307110000000	0.681870000000
	220	0.389320000000	0.360870000000	0.082380000000
	220	0.155700000000	0.379330000000	0.331750000000
	220	0.103940000000	0.408220000000	0.056080000000
	220	0.121520000000	0.427690000000	0.552830000000
	220	0.111070000000	0.413890000000	0.799980000000
295	220	0.356570000000	0.473780000000	0.318130000000
	15	0.380480000000	0.140830000000	0.100450000000
	15	0.378910000000	0.132640000000	0.544350000000
	15	0.115050000000	0.196570000000	0.696290000000
	15	0.124650000000	0.205700000000	0.155340000000
300	15	0.119520000000	0.307500000000	0.899550000000
	15	0.121090000000	0.299310000000	0.455650000000
	15	0.384950000000	0.363230000000	0.303710000000
	15	0.375350000000	0.372370000000	0.844660000000
	15	0.380480000000	0.474170000000	0.100450000000
305	15	0.378910000000	0.465970000000	0.544350000000
	15	0.115050000000	0.529900000000	0.696290000000
	15	0.124650000000	0.539040000000	0.155340000000
	8	0.260240000000	0.107140000000	0.041110000000
	8	0.347510000000	0.185360000000	0.027040000000
310	8	0.500890000000	0.109160000000	0.133790000000
	8	0.421320000000	0.161580000000	0.211770000000
	8	0.314710000000	0.126700000000	0.601830000000
	8	0.305380000000	0.109670000000	0.430770000000
	8	0.398770000000	0.188920000000	0.540190000000
315	8	0.522160000000	0.111680000000	0.618550000000
	8	0.999700000000	0.233380000000	0.640880000000
	8	0.120280000000	0.169240000000	0.612980000000
	8	0.243400000000	0.229850000000	0.760110000000
	8	0.116140000000	0.164340000000	0.779480000000
320	8	0.988590000000	0.221810000000	0.124310000000
	8	0.118860000000	0.148940000000	0.150370000000
	8	0.134250000000	0.228130000000	0.066920000000
	8	0.248920000000	0.220420000000	0.266220000000
	8	0.239760000000	0.273810000000	0.958890000000
325	8	0.152490000000	0.352020000000	0.972960000000
	8	0.999110000000	0.275830000000	0.866210000000
	8	0.078680000000	0.328240000000	0.788230000000
	8	0.194620000000	0.276340000000	0.569230000000
	8	0.185290000000	0.293360000000	0.398170000000
330	8	0.101230000000	0.355580000000	0.459810000000
	8	0.977840000000	0.278340000000	0.381450000000
	8	0.500300000000	0.400050000000	0.359120000000
	8	0.379720000000	0.335910000000	0.387020000000
	8	0.256600000000	0.396520000000	0.239890000000
335	8	0.383860000000	0.331010000000	0.220520000000
	8	0.511410000000	0.388470000000	0.875690000000
	8	0.381140000000	0.315600000000	0.849630000000
	8	0.365750000000	0.394790000000	0.933080000000
	8	0.251080000000	0.387080000000	0.733780000000
340	8	0.260240000000	0.440470000000	0.041110000000
	8	0.347510000000	0.518690000000	0.027040000000
	8	0.500890000000	0.442490000000	0.133790000000
	8	0.421320000000	0.494910000000	0.211770000000
	8	0.314710000000	0.460030000000	0.601830000000
345	8	0.305380000000	0.443000000000	0.430770000000
	8	0.398770000000	0.522250000000	0.540190000000
	8	0.522160000000	0.445010000000	0.618550000000
	8	0.999700000000	0.566720000000	0.640880000000
	8	0.120280000000	0.502570000000	0.612980000000
350	8	0.243400000000	0.563180000000	0.760110000000
	8	0.116140000000	0.497670000000	0.779480000000
	8	0.988590000000	0.555140000000	0.124310000000
	8	0.118860000000	0.482270000000	0.150370000000
	8	0.134250000000	0.561460000000	0.066920000000
355	8	0.248920000000	0.553750000000	0.266220000000

END

8 3

0 0 3 2.0 1.

```

360      0.3220370000D+03  0.5923939339D-01
      0.4843080000D+02  0.3514999608D+00
      0.1042060000D+02  0.7076579210D+00
    0 1 2 6.0 1.
      0.7402940000D+01 -0.4044535832D+00  0.2445861070D+00
      0.1576200000D+01  0.1221561761D+01  0.8539553735D+00
365 0 1 1 0.0 1.
      0.3736840000D+00  0.1000000000D+01  0.1000000000D+01
    220 2
    HAYWSC
    0 1 3 8. 1.
370 5.3568 -1.4687 -0.0794
      1.71 -1.8752 0.2902
      1.0 3.4301 0.1427
    0 1 1 2. 1.
      0.500 1.0 1.0
375 15 5
    0 0 3 2.0 1.
      0.1054900000D+04  0.6554071355D-01
      0.1591950000D+03  0.3840360794D+00
      0.3453040000D+02  0.6745411394D+00
380 0 1 3 8.0 1.
      0.4428660000D+02 -0.1021300535D+00  0.1108510025D+00
      0.1010190000D+02  0.8159224271D-01  0.4564950104D+00
      0.2739970000D+01  0.9697885076D+00  0.6069360139D+00
    0 1 2 5.0 1.
385 0.1218650000D+01 -0.3714960219D+00  0.9158231022D-01
      0.3955460000D+00  0.1270993496D+01  0.9349241043D+00
    0 1 1 0.0 1.
      0.1228110000D+00  0.1000000000D+01  0.1000000000D+01
    0 3 1 0.0 1.
390 0.5500000000D+00  0.1000000000D+01
    99 0
    END
    DFT
    B3LYP
395 XLGRID
    END
    SCFDIR
    TOLINTEG
    6 6 6 6 14
400 SHRINK
    1 1
    LEVSHIFT
    6 1
    FMIXING
405 30
    END
    
```

5) CRYSTAL06 input for the optimization of β -tricalciumphosphate (B3LYP)

```

410 BETA TRICALCIUMPHOSPHATE
    CRYSTAL
    0 0 0
    1
    10.28437400000  10.28440300000  38.61338100000  90.000917  89.999955  120.000372
415 273
      220 0.727720000000  0.860750000000  0.168650000000
      220 0.620370000000  0.815580000000  0.968330000000
      220 0.739980000000  0.861570000000  0.062310000000
      220 0.002300000000  0.001370000000  0.737060000000
420 15 0.002290000000  0.001360000000  0.002780000000
      15 0.689810000000  0.853710000000  0.870410000000
      15 0.653960000000  0.842720000000  0.770240000000
      8 0.727550000000  0.885680000000  0.908400000000
      8 0.751520000000  0.755910000000  0.855460000000
425 8 0.736490000000  0.007530000000  0.852000000000
      8 0.515170000000  0.759490000000  0.862150000000
      8 0.600630000000  0.951110000000  0.782910000000
      8 0.578540000000  0.684610000000  0.785530000000
      8 0.083490000000  0.906150000000  0.779210000000
430 8 0.624300000000  0.825220000000  0.730490000000
    
```

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	8	0.008070000000	0.859940000000	0.991330000000
	8	0.002290000000	0.001360000000	0.043190000000
	220	0.142890000000	0.867400000000	0.168650000000
	220	0.188080000000	0.805230000000	0.968330000000
435	220	0.142090000000	0.878840000000	0.062310000000
	15	0.149900000000	0.836500000000	0.870410000000
	15	0.160930000000	0.811670000000	0.770240000000
	8	0.117940000000	0.842250000000	0.908400000000
440	8	0.247670000000	0.996010000000	0.855470000000
	8	0.996090000000	0.729330000000	0.852000000000
	8	0.244140000000	0.756090000000	0.862150000000
	8	0.052520000000	0.649940000000	0.782900000000
	8	0.319030000000	0.894350000000	0.785540000000
445	8	0.097500000000	0.177780000000	0.779200000000
	8	0.178450000000	0.799530000000	0.730490000000
	8	0.143700000000	0.148560000000	0.991330000000
	220	0.136250000000	0.275920000000	0.168650000000
	220	0.198430000000	0.383280000000	0.968340000000
450	220	0.124820000000	0.263690000000	0.062310000000
	15	0.167130000000	0.313840000000	0.870400000000
	15	0.191980000000	0.349700000000	0.770230000000
	8	0.161340000000	0.276110000000	0.908400000000
	8	0.007620000000	0.252110000000	0.855460000000
455	8	0.274290000000	0.267180000000	0.852000000000
	8	0.247550000000	0.488480000000	0.862150000000
	8	0.353700000000	0.403040000000	0.782900000000
	8	0.109290000000	0.425120000000	0.785530000000
	8	0.825880000000	0.920170000000	0.779210000000
460	8	0.204120000000	0.379360000000	0.730490000000
	8	0.855080000000	0.995570000000	0.991330000000
	220	0.135800000000	0.861260000000	0.670600000000
	220	0.205170000000	0.819990000000	0.470450000000
	220	0.150840000000	0.844100000000	0.567210000000
465	220	0.002290000000	0.001380000000	0.424590000000
	220	0.002280000000	0.001350000000	0.236430000000
	15	0.002300000000	0.001390000000	0.499870000000
	15	0.166720000000	0.868200000000	0.370630000000
	15	0.186020000000	0.831850000000	0.270600000000
470	8	0.169080000000	0.920100000000	0.408860000000
	8	0.007700000000	0.785850000000	0.357580000000
	8	0.284740000000	0.013960000000	0.351320000000
	8	0.237070000000	0.762170000000	0.365850000000
	8	0.345250000000	0.935790000000	0.285720000000
475	8	0.090370000000	0.675600000000	0.287640000000
	8	0.823050000000	0.907120000000	0.277860000000
	8	0.204590000000	0.808530000000	0.232180000000
	8	0.869230000000	0.856910000000	0.481800000000
	8	0.002370000000	0.001490000000	0.537530000000
480	220	0.728680000000	0.867870000000	0.670600000000
	220	0.618020000000	0.798470000000	0.470450000000
	220	0.696490000000	0.852830000000	0.567210000000
	15	0.704690000000	0.836930000000	0.370630000000
	15	0.649040000000	0.817590000000	0.270600000000
485	8	0.754230000000	0.834560000000	0.408860000000
	8	0.781380000000	0.995940000000	0.357590000000
	8	0.732420000000	0.718900000000	0.351320000000
	8	0.528320000000	0.766580000000	0.365850000000
	8	0.593790000000	0.658380000000	0.285730000000
490	8	0.588410000000	0.913220000000	0.287640000000
	8	0.087290000000	0.180610000000	0.277850000000
	8	0.607170000000	0.799000000000	0.232180000000
	8	0.990880000000	0.134410000000	0.481770000000
	220	0.142380000000	0.274970000000	0.670600000000
495	220	0.183660000000	0.385630000000	0.470450000000
	220	0.159510000000	0.307080000000	0.567200000000
	15	0.135470000000	0.298980000000	0.370630000000
	15	0.171790000000	0.354610000000	0.270600000000
500	8	0.083580000000	0.249440000000	0.408860000000
	8	0.217840000000	0.222340000000	0.357580000000
	8	0.989700000000	0.271220000000	0.351310000000
	8	0.241480000000	0.475360000000	0.365840000000
	8	0.067840000000	0.409880000000	0.285720000000
	8	0.328050000000	0.415230000000	0.287640000000
	8	0.096530000000	0.916360000000	0.277850000000

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505	8	0.195090000000	0.396490000000	0.232180000000
	8	0.146730000000	0.012760000000	0.481780000000
	220	0.061050000000	0.527420000000	0.835320000000
	220	0.953700000000	0.482250000000	0.635000000000
	220	0.073310000000	0.528230000000	0.728980000000
510	220	0.335620000000	0.668040000000	0.403720000000
	15	0.335630000000	0.668030000000	0.669440000000
	15	0.023140000000	0.520390000000	0.537070000000
	15	0.987290000000	0.509390000000	0.436900000000
	8	0.060880000000	0.552350000000	0.575070000000
515	8	0.084860000000	0.422590000000	0.522130000000
	8	0.069810000000	0.674210000000	0.518670000000
	8	0.848500000000	0.426170000000	0.528820000000
	8	0.933960000000	0.617780000000	0.449570000000
	8	0.911870000000	0.351280000000	0.452200000000
520	8	0.416820000000	0.572820000000	0.445870000000
	8	0.957630000000	0.491880000000	0.397160000000
	8	0.341410000000	0.526600000000	0.658000000000
	8	0.335640000000	0.668060000000	0.709860000000
	220	0.476220000000	0.534070000000	0.835310000000
525	220	0.521410000000	0.471900000000	0.635000000000
	220	0.475430000000	0.545520000000	0.728980000000
	15	0.483240000000	0.503170000000	0.537070000000
	15	0.494260000000	0.478340000000	0.436900000000
	8	0.451280000000	0.508930000000	0.575070000000
530	8	0.581010000000	0.662680000000	0.522130000000
	8	0.329420000000	0.396010000000	0.518670000000
	8	0.577470000000	0.422770000000	0.528820000000
	8	0.385860000000	0.316610000000	0.449570000000
	8	0.652360000000	0.561020000000	0.452210000000
535	8	0.430840000000	0.844450000000	0.445870000000
	8	0.511780000000	0.466190000000	0.397160000000
	8	0.477040000000	0.815210000000	0.657980000000
	220	0.469580000000	0.942580000000	0.835320000000
	220	0.531760000000	0.049950000000	0.635000000000
540	220	0.458140000000	0.930360000000	0.728990000000
	15	0.500460000000	0.980510000000	0.537070000000
	15	0.525310000000	0.016360000000	0.436900000000
	8	0.494680000000	0.942780000000	0.575060000000
	8	0.340950000000	0.918790000000	0.522130000000
545	8	0.607620000000	0.933840000000	0.518660000000
	8	0.580880000000	0.155150000000	0.528820000000
	8	0.687040000000	0.069690000000	0.449570000000
	8	0.442640000000	0.091790000000	0.452200000000
	8	0.159210000000	0.586830000000	0.445870000000
550	8	0.537460000000	0.046020000000	0.397160000000
	8	0.188420000000	0.662230000000	0.657990000000
	220	0.469130000000	0.527920000000	0.337270000000
	220	0.538500000000	0.486650000000	0.137110000000
	220	0.484170000000	0.510750000000	0.233880000000
555	220	0.335640000000	0.668060000000	0.091260000000
	220	0.335610000000	0.668020000000	0.903100000000
	15	0.335630000000	0.668060000000	0.166540000000
	15	0.500050000000	0.534850000000	0.037290000000
	15	0.519360000000	0.498520000000	0.937270000000
560	8	0.502370000000	0.586720000000	0.075530000000
	8	0.341040000000	0.452450000000	0.024240000000
	8	0.618050000000	0.680620000000	0.017980000000
	8	0.570440000000	0.428850000000	0.032510000000
	8	0.678580000000	0.602460000000	0.952390000000
565	8	0.423710000000	0.342260000000	0.954310000000
	8	0.156380000000	0.573790000000	0.944520000000
	8	0.537930000000	0.475220000000	0.898850000000
	8	0.202560000000	0.523590000000	0.148470000000
	8	0.335710000000	0.668160000000	0.204190000000
570	220	0.062010000000	0.534520000000	0.337270000000
	220	0.951350000000	0.465140000000	0.137120000000
	220	0.029820000000	0.519490000000	0.233870000000
	15	0.038020000000	0.503610000000	0.037300000000
	15	0.982380000000	0.484260000000	0.937270000000
575	8	0.087580000000	0.501310000000	0.075530000000
	8	0.114630000000	0.662620000000	0.024240000000
	8	0.065800000000	0.385620000000	0.017990000000
	8	0.861630000000	0.433220000000	0.032520000000

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580	8	0.927140000000	0.325050000000	0.952390000000
	8	0.921730000000	0.579870000000	0.954310000000
	8	0.420630000000	0.847280000000	0.944520000000
	8	0.940500000000	0.465650000000	0.898850000000
	8	0.324220000000	0.801080000000	0.148440000000
585	220	0.475720000000	0.941640000000	0.337270000000
	220	0.517010000000	0.052300000000	0.137120000000
	220	0.492840000000	0.973720000000	0.233870000000
	15	0.468800000000	0.965650000000	0.037290000000
	15	0.505130000000	0.021290000000	0.937260000000
590	8	0.416930000000	0.916100000000	0.075530000000
	8	0.551180000000	0.889010000000	0.024240000000
	8	0.323030000000	0.937870000000	0.017980000000
	8	0.574810000000	0.142020000000	0.032510000000
	8	0.401180000000	0.076550000000	0.952380000000
595	8	0.661390000000	0.081900000000	0.954300000000
	8	0.429870000000	0.583030000000	0.944520000000
	8	0.528430000000	0.063170000000	0.898840000000
	8	0.480050000000	0.679430000000	0.148450000000
	220	0.394390000000	0.194090000000	0.501980000000
600	220	0.287030000000	0.148910000000	0.301670000000
	220	0.406640000000	0.194890000000	0.395650000000
	220	0.668950000000	0.334690000000	0.070390000000
	15	0.668960000000	0.334690000000	0.336110000000
	15	0.356470000000	0.187050000000	0.203740000000
605	15	0.320620000000	0.176040000000	0.103570000000
	8	0.394210000000	0.219020000000	0.241730000000
	8	0.418190000000	0.089260000000	0.188800000000
	8	0.403140000000	0.340870000000	0.185330000000
	8	0.181830000000	0.092830000000	0.195490000000
610	8	0.267280000000	0.284420000000	0.116240000000
	8	0.245210000000	0.017930000000	0.118870000000
	8	0.750150000000	0.239480000000	0.112540000000
	8	0.290970000000	0.158540000000	0.063820000000
	8	0.674750000000	0.193270000000	0.324670000000
615	8	0.668960000000	0.334710000000	0.376530000000
	220	0.809550000000	0.200730000000	0.501980000000
	220	0.854740000000	0.138560000000	0.301670000000
	220	0.808760000000	0.212180000000	0.395650000000
	15	0.816570000000	0.169830000000	0.203740000000
620	15	0.827620000000	0.145030000000	0.103570000000
	8	0.784610000000	0.175590000000	0.241730000000
	8	0.914330000000	0.329340000000	0.188800000000
	8	0.662750000000	0.062660000000	0.185330000000
	8	0.910810000000	0.089430000000	0.195480000000
625	8	0.719250000000	0.983300000000	0.116240000000
	8	0.985730000000	0.227750000000	0.118870000000
	8	0.764160000000	0.511110000000	0.112540000000
	8	0.845130000000	0.132880000000	0.063820000000
	8	0.810380000000	0.481880000000	0.324660000000
630	220	0.802920000000	0.609250000000	0.501990000000
	220	0.865090000000	0.716610000000	0.301670000000
	220	0.791470000000	0.597020000000	0.395650000000
	15	0.833790000000	0.647170000000	0.203740000000
	15	0.858630000000	0.683030000000	0.103570000000
635	8	0.828000000000	0.609430000000	0.241730000000
	8	0.674290000000	0.585440000000	0.188790000000
	8	0.940950000000	0.600500000000	0.185330000000
	8	0.914210000000	0.821810000000	0.195480000000
	8	0.020350000000	0.736380000000	0.116240000000
640	8	0.775920000000	0.758430000000	0.118870000000
	8	0.492540000000	0.253490000000	0.112540000000
	8	0.870780000000	0.712680000000	0.063820000000
	8	0.521760000000	0.328900000000	0.324660000000
	220	0.802470000000	0.194590000000	0.003930000000
645	220	0.871840000000	0.153320000000	0.803780000000
	220	0.817530000000	0.177410000000	0.900550000000
	220	0.668960000000	0.334730000000	0.757920000000
	220	0.668950000000	0.334690000000	0.569760000000
	15	0.668970000000	0.334730000000	0.833210000000
650	15	0.833380000000	0.201520000000	0.703960000000
	15	0.852690000000	0.165190000000	0.603930000000
	8	0.835710000000	0.253410000000	0.742190000000
	8	0.674370000000	0.119130000000	0.690910000000

8	0.951380000000	0.347290000000	0.684650000000	
8	0.903760000000	0.095520000000	0.699180000000	
655	8	0.011920000000	0.269130000000	0.619050000000
8	0.757050000000	0.008940000000	0.620970000000	
8	0.489710000000	0.240460000000	0.611190000000	
8	0.871270000000	0.141880000000	0.565510000000	
8	0.535880000000	0.190230000000	0.815150000000	
660	8	0.669060000000	0.334890000000	0.870860000000
220	0.395340000000	0.201190000000	0.003930000000	
220	0.284680000000	0.131800000000	0.803780000000	
220	0.363170000000	0.186170000000	0.900540000000	
665	15	0.371370000000	0.170260000000	0.703970000000
15	0.315710000000	0.150940000000	0.603940000000	
8	0.420900000000	0.167890000000	0.742200000000	
8	0.448070000000	0.329280000000	0.690920000000	
8	0.399100000000	0.052230000000	0.684650000000	
670	8	0.195000000000	0.099930000000	0.699180000000
8	0.260460000000	0.991720000000	0.619060000000	
8	0.255080000000	0.246560000000	0.620980000000	
8	0.753960000000	0.513950000000	0.611180000000	
8	0.273830000000	0.132340000000	0.565520000000	
8	0.657540000000	0.467720000000	0.815100000000	
675	220	0.809070000000	0.608300000000	0.003930000000
220	0.850330000000	0.718960000000	0.803780000000	
220	0.826170000000	0.640380000000	0.900530000000	
15	0.802140000000	0.632320000000	0.703960000000	
15	0.838460000000	0.687950000000	0.603930000000	
680	8	0.750260000000	0.582790000000	0.742190000000
8	0.884500000000	0.555680000000	0.690910000000	
8	0.656370000000	0.604560000000	0.684650000000	
8	0.908150000000	0.808700000000	0.699180000000	
685	8	0.734510000000	0.743220000000	0.619050000000
8	0.994720000000	0.748570000000	0.620970000000	
8	0.763200000000	0.249700000000	0.611190000000	
8	0.861760000000	0.729840000000	0.565510000000	
8	0.813380000000	0.346080000000	0.815110000000	
END				
690	8 3			
0 0 3	2.0 1.			
	0.3220370000D+03	0.5923939339D-01		
	0.4843080000D+02	0.3514999608D+00		
	0.1042060000D+02	0.7076579210D+00		
695	0 1 2	6.0 1.		
	0.7402940000D+01	-0.4044535832D+00	0.2445861070D+00	
	0.1576200000D+01	0.1221561761D+01	0.8539553735D+00	
0 1 1	0.0 1.			
	0.3736840000D+00	0.1000000000D+01	0.1000000000D+01	
700	220 2			
HAYWSC				
0 1 3	8. 1.			
5.3568	-1.4687	-0.0794		
1.71	-1.8752	0.2902		
705	1.0	3.4301	0.1427	
0 1 1	2. 1.			
0.500	1.0	1.0		
15 5				
0 0 3	2.0 1.			
710	0.1054900000D+04	0.6554071355D-01		
	0.1591950000D+03	0.3840360794D+00		
	0.3453040000D+02	0.6745411394D+00		
0 1 3	8.0 1.			
	0.4428660000D+02	-0.1021300535D+00	0.1108510025D+00	
715	0.1010190000D+02	0.8159224271D-01	0.4564950104D+00	
	0.2739970000D+01	0.9697885076D+00	0.6069360139D+00	
0 1 2	5.0 1.			
	0.1218650000D+01	-0.3714960219D+00	0.9158231022D-01	
	0.3955460000D+00	0.1270993496D+01	0.9349241043D+00	
720	0 1 1	0.0 1.		
	0.1228110000D+00	0.1000000000D+01	0.1000000000D+01	
0 3 1	0.0 1.			
	0.5500000000D+00	0.1000000000D+01		
99 0				
725	END			
DFT				

730 B3LYP
XLGRID
END
SCFDIR
TOLINTEG
6 6 6 6 14
SHRINK
1 1
735 LEVSHIFT
6 1
FMIXING
30
END