Electronic Supporting Information for

Theoretical investigations into the enantiomeric and racemic forms of α-(trifluoromethyl)lactic acid

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The following Tables contain the optimized structures from VASP and Gaussian03 calculations. Structures from periodic boundary condition(PBC)-calculations are given in a fractional coordinate format suitable for VASP (CONTCAR). Structures from non-PBC calculations are given in cartesian coordinates. Length unit is Å throughout and SCF-energies are given in eV for PBC-calculations and a.u. for non-PBC calculations.

Table 1S Solid state structures in CONTCAR-format (VASP) with SCF energies.

1-S

E(SCF)		-352.5372030		
C	O	F	H	
		1.0742630		
		10.8337884	0.0000000	0.0992765
		0.0000000	5.4821278	0.0000000
		-4.1782280	0.0000000	9.2198103
	16	12	12	20
Direct				
		0.3181606	0.5168575	0.3359178
		0.0814258	0.5171818	0.2602616
		0.1885236	0.4974879	0.2139981
		0.1850919	0.2692728	0.1414223
		0.6818394	0.5168575	0.6640822
		0.9185742	0.5171818	0.7397384
		0.8114764	0.4974879	0.7860019
		0.8149081	0.2692728	0.8585777
		0.8181606	0.0168575	0.3359178
		0.5814258	0.0171818	0.2602616
		0.6885236	0.9974879	0.2139981
		0.6850919	0.7692728	0.1414223
		0.1818394	0.0168575	0.6640822
		0.4185742	0.0171818	0.7397384
		0.3114764	0.9974879	0.7860019
		0.3149081	0.7692728	0.8585777
		0.1790419	0.6793462	0.1244129
		0.1703535	0.0931613	0.2081254

0.1957317	0.2653678	0.0334084
0.8209581	0.6793462	0.8755871
0.8296465	0.0931613	0.7918746
0.8042683	0.2653678	0.9665916
0.6790419	0.1793462	0.1244129
0.6703535	0.5931613	0.2081254
0.6957317	0.7653678	0.0334084
0.3209581	0.1793462	0.8755871
0.3296465	0.5931613	0.7918746
0.3042683	0.7653678	0.9665916
0.3309747	0.7227760	0.3970245
0.4143019	0.4973665	0.2945247
0.3352893	0.3550071	0.4306103
0.6690253	0.7227760	0.6029755
0.5856981	0.4973665	0.7054753
0.6647107	0.3550071	0.5693897
0.8309747	0.2227760	0.3970245
0.9143019	0.9973665	0.2945247
0.8352893	0.8550071	0.4306103
0.1690253	0.2227760	0.6029755
0.0856981	0.9973665	0.7054753
0.1647107	0.8550071	0.5693897
0.2276448	0.6495133	0.0693135
0.1744313	0.9406643	0.1655050
0.9917355	0.5010102	0.1725899
0.0850869	0.6831161	0.3073845
0.0877918	0.3829711	0.3323709
0.7723552	0.6495133	0.9306865
0.8255687	0.9406643	0.8344950
0.0082645	0.5010102	0.8274101
0.9149131	0.6831161	0.6926155
0.9122082	0.3829711	0.6676291
0.7276448	0.1495133	0.0693135
0.6744313	0.4406643	0.1655050
0.4917355	0.0010102	0.1725899
0.5850869	0.1831161	0.3073845
0.5877918	0.8829711	0.3323709
0.2723552	0.1495133	0.9306865
0.3255687	0.4406643	0.8344950
0.5082645	0.0010102	0.8274101
0.4149131	0.1831161	0.6926155
0.4122082	0.8829711	0.6676291

1-rac (2 molecules in unit cell)

E(SCF) -176.2688730

C	O	F	H	
		1.0452910		
		5.6147519	0.0111520	-0.0591937
		-2.5657018	5.5054383	-0.0790758
		-0.3992531	-1.2320859	9.4590824
	8	6	6	10
Direct				
		0.3518576	0.2986006	0.1668785
		0.1632953	0.8934588	0.2375144
		0.3125398	0.1556099	0.2877059
		0.5761522	0.2135898	0.3608852
		0.6481424	0.7013994	0.8331215
		0.8367047	0.1065412	0.7624856
		0.6874602	0.8443901	0.7122941
		0.4238478	0.7864102	0.6391148
		0.1716122	0.2275321	0.3786059
		0.6569516	0.3411641	0.4711713
		0.6977080	0.1120133	0.2921692
		0.8283878	0.7724679	0.6213941
		0.3430484	0.6588359	0.5288287
		0.3022920	0.8879867	0.7078308
		0.4943046	0.5328902	0.2110097
		0.4697143	0.2312282	0.0689694
		0.1264966	0.2750136	0.1073841
		0.5056954	0.4671098	0.7889903
		0.5302857	0.7687718	0.9310306
		0.8735034	0.7249864	0.8926159
		0.2746963	0.3848382	0.4320915
		0.8780807	0.1640912	0.3352960
		0.1418077	0.7973871	0.3242660
		0.2620552	0.8323473	0.1638361
		0.9758058	0.8585806	0.1899505
		0.7253037	0.6151618	0.5679085
		0.1219193	0.8359088	0.6647040
		0.8581923	0.2026129	0.6757340
		0.7379448	0.1676527	0.8361639
		0.0241942	0.1414194	0.8100495

1-rac (4 molecules in 211-super cell)

E(SCF)	-352.5345170			
C	O	F	H	
		11.7387747		
		0.9997541	-0.0005463	-0.0038822
		-0.2276078	0.4895020	-0.0007948

	-0.0479500	-0.1284609	0.8426741
16	12	12	20
Direct			
	0.1785829	0.3034063	0.1497948
	0.0840777	0.8984396	0.2209517
	0.1596706	0.1619489	0.2706299
	0.2922050	0.2211101	0.3437093
	0.3340310	0.7209564	0.8126842
	0.4277359	0.1255576	0.7410813
	0.3521851	0.8619535	0.6917219
	0.2194130	0.8024089	0.6190954
	0.6780512	0.3047703	0.1482355
	0.5843463	0.9001691	0.2198384
	0.6598971	0.1637733	0.2691978
	0.7926691	0.2233180	0.3418243
	0.8334993	0.7223204	0.8111249
	0.9280045	0.1272873	0.7399680
	0.8524117	0.8637780	0.6902899
	0.7198773	0.8046168	0.6172103
	0.0901055	0.2356909	0.3609995
	0.3340511	0.3519085	0.4531189
	0.3519637	0.1169951	0.2758998
	0.4213596	0.7880889	0.6008483
	0.1771384	0.6705363	0.5100801
	0.1600021	0.9076269	0.6865967
	0.5907226	0.2376379	0.3600714
	0.8349438	0.3551904	0.4508396
	0.8520801	0.1180998	0.2743230
	0.9219767	0.7900360	0.5999202
	0.6780311	0.6738184	0.5078008
	0.6601185	0.9087317	0.6850199
	0.2503310	0.5390234	0.1934605
	0.2368159	0.2344983	0.0525688
	0.0653718	0.2787158	0.0901114
	0.2624550	0.4851935	0.7693851
	0.2760289	0.7898241	0.9102089
	0.4475605	0.7463872	0.8718782
	0.7496272	0.5405334	0.1915346
	0.7360533	0.2359027	0.0507107
	0.5645218	0.2793397	0.0890416
	0.7617510	0.4867033	0.7674592
	0.7752663	0.7912286	0.9083509
	0.9467104	0.7470110	0.8708083
	0.1423034	0.3942093	0.4140920
	0.4428473	0.1707818	0.3184430

0.0737016	0.8034118	0.3076560
0.1327026	0.8356619	0.1477645
0.4899948	0.8645481	0.1727394
0.3691072	0.6290472	0.5483921
0.0693353	0.8546420	0.6435857
0.4374496	0.2203027	0.6543265
0.3793962	0.1882826	0.8146557
0.0221057	0.1624709	0.7876133
0.6429750	0.3966797	0.4125276
0.9427468	0.1710849	0.3173340
0.5746326	0.8054241	0.3065932
0.6326860	0.8374441	0.1462640
0.9899765	0.8632559	0.1733064
0.8697789	0.6315176	0.5468277
0.5692349	0.8549451	0.6424767
0.9383806	0.2223150	0.6532637
0.8793795	0.1900648	0.8131552
0.5220874	0.1611788	0.7881803

Table S2 Free molecules α-(trifluoromethyl)lactic acid in CONTCAR and xyz-format with SCF energies.

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VASP (PBE)	E(SCF)		-87.5955400	
C	O	F	H	
		3.0000000		
		5.8633000	0.0000000	0.0000000
		-2.6897064	5.3483511	0.0000000
		-0.2110511	-0.6790812	6.3664073
	4	3	3	5
Direct				
		0.2216136	0.2405128	0.4243129
		0.2890897	0.3841653	0.3807974
		0.2364031	0.2901663	0.3590251
		0.1491207	0.2690779	0.3215071
		0.2808820	0.2619063	0.3127362
		0.1248103	0.2267736	0.2648627
		0.1045091	0.3024517	0.3562680
		0.1723588	0.1567675	0.4061916
		0.1819942	0.2655611	0.4741526
		0.2970637	0.2510715	0.4547380
		0.2384063	0.2246437	0.2750790
		0.0503961	0.2848165	0.3282502
		0.2972231	0.4180104	0.3343120
		0.2582037	0.4071551	0.4196706
		0.3523255	0.3958870	0.4027966
G03 (PBE)				
E(SCF)			-680.2231180	
F		1.8693250	4.2681780	3.9142420
F		3.2600770	2.8921340	2.9376820
F		1.7174570	2.1212540	4.2863160
O		1.3040750	3.9950620	1.2308920
H		1.8216110	3.5848920	0.5061060
O		0.8468620	0.5253530	2.0621270
H		1.0828110	-0.2498260	1.5123100
O		1.8034760	1.5765810	0.2977150
C		1.9729300	3.0536990	3.3337130
C		-0.4498150	3.0662310	2.5885950
H		-1.1163450	2.9682610	1.7233490
H		-0.5946600	4.0601920	3.0284060
H		-0.6995450	2.2989710	3.3293840
C		1.0009820	2.9444960	2.1196000
C		1.2687600	1.6125220	1.3895630

Table S3 Cartesian coordinates and SCF energies of Dimer **A-RS** at level of theory given in header

BP86

E(SCF)	-1361.8778482		
F	-1.6234100	-3.9106300	-4.4241500
F	-3.1562500	-3.0084700	-3.1475700
F	-1.7383700	-1.7356600	-4.2307900
O	-1.0572000	-4.2660600	-1.7394000
H	-1.6817500	-4.1419400	-0.9952600
O	-0.9643200	-0.6803200	-1.6337700
H	-1.2862400	-0.0212400	-0.9130600
O	-1.8888500	-2.2443500	-0.2758900
C	-1.8625300	-2.9057400	-3.5538900
C	0.5605600	-2.8364700	-2.7936700
H	1.2235700	-2.8917700	-1.9216900
H	0.8073100	-3.6618400	-3.4720500
H	0.7145500	-1.8811700	-3.3068200
C	-0.8905000	-2.9954700	-2.3319200
C	-1.2958700	-1.9067700	-1.3129900
H	-2.3656400	-1.2066000	0.8198300
O	-2.6875500	-0.5475200	1.5405300
C	-2.3560100	0.6789200	1.2197500
O	-1.7630300	1.0165100	0.1826500
C	-2.7613800	1.7676200	2.2386900
C	-4.2124300	1.6086200	2.7004300
O	-2.5946800	3.0382100	1.6461600
C	-1.7893500	1.6779000	3.4606500
F	-1.9135000	0.5078100	4.1375500
F	-2.0284600	2.6827800	4.3309100
F	-0.4956200	1.7806200	3.0543300
H	-1.9701300	2.9141000	0.9020200
H	-4.8754500	1.6639300	1.8284500
H	-4.4591800	2.4339900	3.3788100
H	-4.3664300	0.6533200	3.2135800

MP2

E(SCF)	-1355.1748753		
F	-1.6095057	-3.8760352	-4.3948956
F	-3.1256781	-3.0216262	-3.1118726
F	-1.7475021	-1.7332896	-4.1702937
O	-1.0454082	-4.2496318	-1.7389612
H	-1.7010334	-4.1441219	-1.0347567

O	-0.9194177	-0.6988611	-1.6371364
H	-1.2361589	-0.0594026	-0.9360148
O	-1.9094038	-2.2247364	-0.3041409
C	-1.8550291	-2.8992971	-3.5232195
C	0.5430964	-2.8252271	-2.7897884
H	1.1989598	-2.8573744	-1.9238544
H	0.7906697	-3.6551750	-3.4457938
H	0.6832915	-1.8856669	-3.3145656
C	-0.8920254	-2.9870714	-2.3266930
C	-1.2909757	-1.9108790	-1.3184538
H	-2.4163979	-1.1683261	0.8424498
O	-2.7329152	-0.5288988	1.5437027
C	-2.3613560	0.6831181	1.2250181
O	-1.7432344	0.9970233	0.2105333
C	-2.7598503	1.7592411	2.2335102
C	-4.1948257	1.5975095	2.6970960
O	-2.6065229	3.0218501	1.6458687
C	-1.7964312	1.6712162	3.4296862
F	-1.9039178	0.5051767	4.0767093
F	-2.0414772	2.6479276	4.3015246
F	-0.5259085	1.7933650	3.0178908
H	-1.9511765	2.9163346	0.9414052
H	-4.8509959	1.6298881	1.8314032
H	-4.4420549	2.4273809	3.3533283
H	-4.3349550	0.6578813	3.2217690

M05-2X

E(SCF) -1361.7847102

F	-1.6091600	-3.8701500	-4.3777000
F	-3.1208700	-3.0151500	-3.0898600
F	-1.7470400	-1.7280400	-4.1542500
O	-1.0504800	-4.2393300	-1.7308600
H	-1.7216800	-4.1655500	-1.0417100
O	-0.9174400	-0.6961700	-1.6260700
H	-1.2309700	-0.0402900	-0.9345600
O	-1.9038100	-2.2058900	-0.3048600
C	-1.8514900	-2.8933000	-3.5057500
C	0.5433900	-2.8189900	-2.7867200
H	1.2021500	-2.8561000	-1.9250000
H	0.7805000	-3.6463300	-3.4474300
H	0.6758100	-1.8772800	-3.3067900
C	-0.8892000	-2.9820500	-2.3157400
C	-1.2859100	-1.9004300	-1.3127200
H	-2.4209000	-1.1875600	0.8413300

O	-2.7344400	-0.5316700	1.5328400
C	-2.3659600	0.6725800	1.2194800
O	-1.7480600	0.9780400	0.2116200
C	-2.7626700	1.7542000	2.2225000
C	-4.1952600	1.5911500	2.6934800
O	-2.6013900	3.0114800	1.6376300
C	-1.8003900	1.6654400	3.4125200
F	-1.9048500	0.5001900	4.0610200
F	-2.0427200	2.6423000	4.2844700
F	-0.5310000	1.7872900	2.9966400
H	-1.9301900	2.9377000	0.9484800
H	-4.8540200	1.6282600	1.8317500
H	-4.4323800	2.4184900	3.3541800
H	-4.3276900	0.6494300	3.2135500

B3LYP

E(SCF)	-1361.8734441		
F	-1.6119900	-3.9114600	-4.4264700
F	-3.1359200	-3.0254600	-3.1620900
F	-1.7356800	-1.7578100	-4.2320200
O	-1.0517700	-4.2646900	-1.7591400
H	-1.6842500	-4.1729700	-1.0328600
O	-0.9609400	-0.6978000	-1.6610000
H	-1.2664900	-0.0453600	-0.9655900
O	-1.8742800	-2.2346300	-0.3017500
C	-1.8540200	-2.9180800	-3.5633300
C	0.5585500	-2.8445600	-2.8039600
H	1.2129800	-2.8914900	-1.9357100
H	0.8075000	-3.6689900	-3.4684000
H	0.7130500	-1.9009500	-3.3198300
C	-0.8899400	-3.0018800	-2.3474600
C	-1.2925800	-1.9166000	-1.3312600
H	-2.3853900	-1.1824900	0.8723600
O	-2.6909300	-0.5300500	1.5677700
C	-2.3592900	0.6887600	1.2380200
O	-1.7776000	1.0067800	0.2085200
C	-2.7619300	1.7740300	2.2542200
C	-4.2104200	1.6167100	2.7107200
O	-2.6001000	3.0368400	1.6659100
C	-1.7978600	1.6902300	3.4700900
F	-1.9162000	0.5299600	4.1387800
F	-2.0398900	2.6836100	4.3332300
F	-0.5159600	1.7976100	3.0688600

H	-1.9676200	2.9451200	0.9396300
H	-4.8648600	1.6636400	1.8424700
H	-4.4593800	2.4411400	3.3751600
H	-4.3649300	0.6731000	3.2265900

PBE

E(SCF)	-1360.4741630		
F	-1.6229900	-3.9031100	-4.4172800
F	-3.1523200	-3.0059600	-3.1373200
F	-1.7381300	-1.7310700	-4.2179500
O	-1.0557700	-4.2633500	-1.7373700
H	-1.6829600	-4.1396900	-0.9967400
O	-0.9595700	-0.6827200	-1.6317900
H	-1.2822700	-0.0247500	-0.9137900
O	-1.8895200	-2.2430500	-0.2759300
C	-1.8614100	-2.9016500	-3.5457900
C	0.5575400	-2.8348400	-2.7915900
H	1.2230600	-2.8933300	-1.9221200
H	0.8014200	-3.6577300	-3.4736900
H	0.7097300	-1.8779800	-3.3018600
C	-0.8895900	-2.9946200	-2.3271500
C	-1.2935300	-1.9071700	-1.3104500
H	-2.3696000	-1.2031000	0.8205500
O	-2.6923000	-0.5451200	1.5385500
C	-2.3583400	0.6793200	1.2172100
O	-1.7623600	1.0152000	0.1826900
C	-2.7622900	1.7667700	2.2339200
C	-4.2094200	1.6069900	2.6983600
O	-2.5961100	3.0355000	1.6441300
C	-1.7904600	1.6738000	3.4525500
F	-1.9137400	0.5032300	4.1247000
F	-2.0288800	2.6752600	4.3240400
F	-0.4995500	1.7781200	3.0440700
H	-1.9689200	2.9118400	0.9035000
H	-4.8749400	1.6654800	1.8289000
H	-4.4532900	2.4298800	3.3804600
H	-4.3616000	0.6501300	3.2086300

LDA

E(SCF)	-1352.1986286		
F	-1.6463700	-3.8150900	-4.3027000
F	-3.1408400	-2.9055600	-3.0373500
F	-1.7225200	-1.6695000	-4.1005300

O	-1.1083000	-4.1798500	-1.6660200
H	-1.6806400	-4.0255400	-0.8804000
O	-1.0139900	-0.6517000	-1.5692400
H	-1.3485500	0.0516800	-0.8287500
O	-1.8830700	-2.2197900	-0.2179800
C	-1.8690800	-2.8240700	-3.4454600
C	0.5067100	-2.7751500	-2.7138000
H	1.1849200	-2.8737700	-1.8546300
H	0.7328400	-3.5755900	-3.4328600
H	0.6566300	-1.7966300	-3.1898000
C	-0.9157300	-2.9365100	-2.2468800
C	-1.3067100	-1.8563700	-1.2575800
H	-2.3033300	-1.2795300	0.7355200
O	-2.6378800	-0.5761500	1.4760000
C	-2.3451700	0.6285200	1.1643500
O	-1.7688100	0.9919400	0.1247500
C	-2.7361400	1.7086600	2.1536500
C	-4.1585900	1.5473000	2.6205600
O	-2.5435800	2.9520100	1.5727800
C	-1.7828000	1.5962200	3.3522300
F	-1.9293600	0.4416500	4.0072900
F	-2.0055100	2.5872500	4.2094700
F	-0.5110300	1.6777100	2.9441100
H	-1.9712300	2.7976900	0.7871600
H	-4.8368000	1.6459300	1.7613900
H	-4.3847200	2.3477500	3.3396200
H	-4.3085100	0.5687800	3.0965600

PW91

E(SCF)	-1361.4880281		
F	-1.6243000	-3.8980400	-4.4104400
F	-3.1520300	-3.0013000	-3.1309200
F	-1.7390100	-1.7276000	-4.2112300
O	-1.0579200	-4.2576500	-1.7328200
H	-1.6836900	-4.1351300	-0.9921000
O	-0.9612500	-0.6805400	-1.6263600
H	-1.2835800	-0.0209200	-0.9091100
O	-1.8908200	-2.2401500	-0.2737300
C	-1.8622000	-2.8973700	-3.5396100
C	0.5548200	-2.8306200	-2.7867800
H	1.2191800	-2.8900400	-1.9187000
H	0.7976100	-3.6518000	-3.4685500
H	0.7067200	-1.8747500	-3.2953500
C	-0.8912200	-2.9899700	-2.3225500

C	-1.2947300	-1.9035800	-1.3069200
H	-2.3682900	-1.2069300	0.8158700
O	-2.6906200	-0.5473100	1.5331300
C	-2.3571500	0.6757300	1.2136800
O	-1.7610600	1.0123100	0.1804900
C	-2.7606600	1.7621200	2.2293100
C	-4.2067000	1.6027700	2.6935500
O	-2.5939600	3.0298000	1.6395900
C	-1.7896800	1.6695300	3.4463800
F	-1.9128600	0.4997500	4.1179900
F	-2.0275700	2.6701900	4.3172100
F	-0.4998400	1.7734500	3.0376800
H	-1.9681900	2.9072800	0.8988600
H	-4.8710600	1.6621900	1.8254600
H	-4.4494900	2.4239500	3.3753100
H	-4.3586000	0.6469100	3.2021100

Table S4 Cartesian coordinates and SCF energies of Dimer **A-SS** at level of theory given in header

PW91

E(SCF)	-1361.4878992		
F	1.7083500	4.1446000	4.3177600
F	3.1688600	3.1231700	3.0534300
F	1.8080400	1.9641500	4.3149200
O	1.0137500	4.2565000	1.6458000
H	1.6110500	4.0614100	0.8972500
O	0.8880700	0.6869800	1.8832100
H	1.1692700	-0.0408200	1.2164100
O	1.7653100	2.1008200	0.3478100
C	1.9011400	3.0659500	3.5327600
C	-0.5504800	2.9526600	2.9099200
H	-1.2575700	2.9373300	2.0742800
H	-0.7537000	3.8365900	3.5226100
H	-0.6818000	2.0503600	3.5132400
C	0.8711500	3.0523000	2.3615400
C	1.2168600	1.8703700	1.4350400
H	2.1760000	0.9639200	-0.6633600
O	2.4450400	0.2370500	-1.3361800
C	2.1419600	-0.9483200	-0.8753000
O	1.5826100	-1.1779300	0.2065500
C	2.5217400	-2.1328800	-1.7849500
C	2.1153400	-1.8924300	-3.2370800
O	1.8928700	-3.2996200	-1.3096100
C	4.0637900	-2.3446300	-1.6845800
F	4.7622500	-1.2894600	-2.1674600
F	4.4360800	-3.4371200	-2.3808300
F	4.4377400	-2.5283100	-0.3936200
H	1.6830700	-3.1343800	-0.3694900
H	1.0324700	-1.7392300	-3.2863800
H	2.3691100	-2.7802600	-3.8247800
H	2.6248700	-1.0192600	-3.6534200

BP86

E(SCF)	-1361.8777186		
F	1.7009200	4.1569100	4.3331800
F	3.1702000	3.1281200	3.0779300
F	1.7973800	1.9723100	4.3364200
O	1.0174700	4.2660100	1.6517700
H	1.6158800	4.0682700	0.9021700

O	0.8893900	0.6879900	1.8893100
H	1.1719100	-0.0398900	1.2201700
O	1.7685900	2.1049200	0.3518100
C	1.8964000	3.0739600	3.5496100
C	-0.5591700	2.9618100	2.9096300
H	-1.2616700	2.9434500	2.0675000
H	-0.7675800	3.8498000	3.5181600
H	-0.6963500	2.0605700	3.5167200
C	0.8700300	3.0591500	2.3695000
C	1.2192700	1.8743300	1.4408900
H	2.1804300	0.9624400	-0.6636200
O	2.4505300	0.2355200	-1.3389000
C	2.1475300	-0.9528900	-0.8771900
O	1.5872300	-1.1826400	0.2064500
C	2.5265200	-2.1400100	-1.7911000
C	2.1087700	-1.9004100	-3.2443400
O	1.8986400	-3.3098600	-1.3108900
C	4.0732800	-2.3530200	-1.6990800
F	4.7718500	-1.2975400	-2.1894800
F	4.4423000	-3.4493200	-2.3968500
F	4.4573100	-2.5348700	-0.4077800
H	1.6890000	-3.1420600	-0.3690900
H	1.0238900	-1.7443700	-3.2858700
H	2.3556500	-2.7913600	-3.8338500
H	2.6176600	-1.0277900	-3.6676700

M05-2X

E(SCF)	-1361.7845567		
F	1.7212400	4.1343100	4.2606100
F	3.1454800	3.1721500	2.9489400
F	1.8788000	1.9819200	4.2360300
O	0.9611100	4.2341500	1.6376500
H	1.5882500	4.0990500	0.9169900
O	0.8646200	0.6981700	1.8948500
H	1.1347600	-0.0219200	1.2505500
O	1.7356800	2.0728800	0.3621700
C	1.9141500	3.0789000	3.4715200
C	-0.5271500	2.9179700	2.9501600
H	-1.2501600	2.8656100	2.1424000
H	-0.7240700	3.8054200	3.5424800
H	-0.6070300	2.0317300	3.5690800
C	0.8629600	3.0412200	2.3562300
C	1.1969700	1.8667300	1.4383100

H	2.1799600	0.9473700	-0.7126100
O	2.4387900	0.2281500	-1.3625000
C	2.1330600	-0.9424600	-0.8927900
O	1.5796500	-1.1474800	0.1760800
C	2.5140000	-2.1205700	-1.7875100
C	2.1654200	-1.8633900	-3.2410300
O	1.8576200	-3.2705000	-1.3449200
C	4.0215600	-2.3553300	-1.6377900
F	4.7400900	-1.3109700	-2.0645300
F	4.3998900	-3.4250200	-2.3352100
F	4.3350600	-2.5675800	-0.3514600
H	1.6803700	-3.1700500	-0.4018300
H	1.0996200	-1.6732500	-3.3176400
H	2.4064300	-2.7542400	-3.8115500
H	2.7161600	-1.0134300	-3.6271600

MP2

E(SCF)	-1355.1747292		
C	1.2630023	1.9613644	1.8981387
C	1.0903244	0.6373264	2.6612085
C	2.2921870	0.4898894	3.5980372
C	1.5482398	3.0012035	8.1491539
C	1.1554614	3.7602225	6.8702037
C	-0.2343221	3.2837991	6.4432225
O	-0.0889522	0.6893418	3.4056506
O	2.2974088	0.8894818	4.7422798
O	3.3337714	-0.1302161	3.0314911
O	2.0854441	3.4726215	5.8718851
O	-0.4248850	2.4877042	5.5515124
O	-1.2225217	3.8432994	7.1529757
F	1.2829725	2.9969554	2.7473521
F	2.4089204	1.9839948	1.2017247
F	0.2597477	2.1540980	1.0419389
F	1.5454837	1.6787464	7.9276112
F	0.7050949	3.2453857	9.1607630
F	2.7726524	3.3466795	8.5469610
H	0.0222957	1.3059296	4.1485629
H	4.0356295	-0.1423022	3.7018113
H	1.9512732	2.5612686	5.5615319
H	-2.0470091	3.4601995	6.8138191
C	1.1838652	5.2569699	7.1196438
H	0.8657776	5.7692032	6.2155126
H	2.2059467	5.5478652	7.3445782

H	0.5304911	5.5345441	7.9403106
C	0.9748683	-0.5158645	1.6832649
H	1.8279958	-0.5555842	1.0138191
H	0.0609878	-0.3884948	1.1106221
H	0.9130995	-1.4464503	2.2404395

PBE

E(SCF)	-1360.4740405		
F	1.7058900	4.1491900	4.3253500
F	3.1686500	3.1258900	3.0624400
F	1.8035900	1.9670300	4.3223200
O	1.0140500	4.2628700	1.6503300
H	1.6132300	4.0662500	0.9023900
O	0.8859900	0.6899100	1.8880900
H	1.1679700	-0.0364400	1.2206800
O	1.7653900	2.1038700	0.3502500
C	1.8990800	3.0696000	3.5398500
C	-0.5537600	2.9586000	2.9121900
H	-1.2608900	2.9432100	2.0743000
H	-0.7581000	3.8442600	3.5251300
H	-0.6870000	2.0553800	3.5168000
C	0.8698400	3.0575300	2.3656000
C	1.2161100	1.8744000	1.4382400
H	2.1780600	0.9594800	-0.6672600
O	2.4472800	0.2341100	-1.3409700
C	2.1435400	-0.9524100	-0.8780800
O	1.5842000	-1.1811100	0.2049400
C	2.5235200	-2.1381400	-1.7887700
C	2.1144400	-1.8980500	-3.2414200
O	1.8958500	-3.3062500	-1.3125200
C	4.0677100	-2.3484200	-1.6907500
F	4.7650800	-1.2922200	-2.1756500
F	4.4400500	-3.4418100	-2.3876900
F	4.4444100	-2.5315200	-0.3994400
H	1.6878400	-3.1397500	-0.3711900
H	1.0297700	-1.7446500	-3.2893800
H	2.3675300	-2.7874700	-3.8302600
H	2.6239600	-1.0238100	-3.6600100

LDA

E(SCF)	-1352.1984637		
F	1.7296700	4.0234100	4.2430000
F	3.1576800	2.9723400	3.0111800
F	1.7503600	1.8670100	4.2228800

O	1.1096200	4.1738600	1.6005500
H	1.6595700	3.9375600	0.8194100
O	0.9168600	0.6553500	1.8161300
H	1.2062600	-0.1192800	1.1295000
O	1.7870200	2.0730700	0.3085300
C	1.9002100	2.9577000	3.4669200
C	-0.5005400	2.9131000	2.8228700
H	-1.2070800	2.9548800	1.9820800
H	-0.6799700	3.7797800	3.4752000
H	-0.6573800	1.9849700	3.3890100
C	0.9075300	2.9920400	2.2955400
C	1.2347700	1.8188900	1.3927100
H	2.1391000	1.0423600	-0.5764000
O	2.4131500	0.2689200	-1.2706300
C	2.1255600	-0.8969500	-0.8322100
O	1.5679800	-1.1507300	0.2493300
C	2.4987900	-2.0736500	-1.7123000
C	2.0813300	-1.8541000	-3.1421700
O	1.9247600	-3.2268200	-1.2012000
C	4.0245100	-2.2332800	-1.6386200
F	4.6668500	-1.1805200	-2.1511000
F	4.4046900	-3.3151400	-2.3110500
F	4.4162200	-2.3749400	-0.3675400
H	1.6658700	-3.0129400	-0.2761600
H	0.9876700	-1.7572300	-3.1913700
H	2.3828400	-2.7301900	-3.7341400
H	2.5493400	-0.9499400	-3.5544600

B3LYP

E(SCF)	-1361.8733104		
F	1.6820400	4.1586800	4.3367300
F	3.1462900	3.1465800	3.0968400
F	1.7869100	1.9951600	4.3375100
O	1.0126400	4.2665600	1.6708300
H	1.6230800	4.1030200	0.9383900
O	0.8861500	0.7080300	1.9143000
H	1.1558700	-0.0108600	1.2716100
O	1.7584300	2.0975700	0.3807600
C	1.8827100	3.0875700	3.5599300
C	-0.5606000	2.9712900	2.9138100
H	-1.2519500	2.9442300	2.0737600
H	-0.7736600	3.8574800	3.5074300
H	-0.6998800	2.0823500	3.5227200
C	0.8678100	3.0671600	2.3832700

C	1.2170900	1.8858100	1.4584200
H	2.2079300	0.9325200	-0.7094000
O	2.4658800	0.2145400	-1.3579000
C	2.1586800	-0.9650600	-0.8902900
O	1.6049400	-1.1758700	0.1812400
C	2.5351000	-2.1485100	-1.8017200
C	2.1100700	-1.9098800	-3.2485800
O	1.9107700	-3.3109700	-1.3263500
C	4.0715700	-2.3654300	-1.7170100
F	4.7636300	-1.3189400	-2.1998000
F	4.4335900	-3.4489700	-2.4140400
F	4.4556700	-2.5513500	-0.4393300
H	1.7176900	-3.1795800	-0.3875700
H	1.0346000	-1.7467300	-3.2820400
H	2.3425800	-2.7975700	-3.8325800
H	2.6176100	-1.0493100	-3.6754300

Table S5 Cartesian coordinates and SCF energies of Dimer **B-SS** at level of theory given in header

B3LYP

E(SCF)	-1361.8579023		
C	1.9177600	1.4945200	1.1298000
C	1.3224800	1.2138300	2.5111900
C	2.4366000	0.8330700	3.5110400
C	1.8754700	2.9849500	8.0984000
C	1.0820100	3.7049900	6.9723200
C	-0.1820500	2.8835400	6.6357200
O	0.6695400	2.3693400	2.9316000
O	2.6371400	1.4098900	4.5509000
O	3.1884200	-0.1947100	3.0998800
O	1.8941000	3.8255200	5.8479300
O	-0.3772800	2.3493700	5.5723300
O	-1.0675200	2.8397600	7.6380400
H	2.6292700	2.3137300	1.2141800
H	2.4182800	0.6204200	0.7233300
H	1.1162100	1.8029000	0.4623500
F	2.1553400	1.7138200	7.7442800
F	1.2066000	2.9396000	9.2638800
F	3.0388700	3.6076200	8.3270300
H	0.3850300	2.3045000	3.8609400
H	3.8531400	-0.3625800	3.7857800
H	2.0627600	2.9614700	5.4310500
H	-1.8198100	2.3055200	7.3395000
C	0.6978300	5.1168800	7.4199300
H	0.1491100	5.6029000	6.6154700
H	1.6083600	5.6822400	7.6053500
H	0.0863000	5.1008800	8.3174600
C	0.2942400	0.0514500	2.4236200
F	0.8172500	-1.0726100	1.9032900
F	-0.7479000	0.4010200	1.6586200
F	-0.1823400	-0.2545800	3.6478500

M05-2X

E(SCF)	-1361.7710291		
C	2.0183600	1.5069200	1.2209400
C	1.3371000	1.2603600	2.5577400
C	2.3565400	0.7804600	3.5913500
C	1.9540000	3.0706000	7.9957500
C	1.0716700	3.6928100	6.9068200

C	-0.1221900	2.7741600	6.6447800
O	0.7528200	2.4471400	2.9760400
O	2.5760900	1.3463400	4.6287500
O	3.0073000	-0.3196200	3.2203700
O	1.8228600	3.8441900	5.7502700
O	-0.3377900	2.2400100	5.5898600
O	-0.9268400	2.6404500	7.6964200
H	2.7755300	2.2726800	1.3574100
H	2.4730400	0.6004000	0.8388500
H	1.2714800	1.8736100	0.5242300
F	2.2918100	1.8153300	7.6615900
F	1.3515700	3.0240500	9.1891800
F	3.0780600	3.7723600	8.1404300
H	0.4186500	2.3728200	3.8860600
H	3.6227100	-0.5485500	3.9302900
H	2.0402200	2.9820200	5.3569000
H	-1.6450300	2.0453600	7.4411100
C	0.5924400	5.0660900	7.3499600
H	-0.0163800	5.4896600	6.5573600
H	1.4636600	5.6963000	7.4967000
H	0.0170000	5.0043400	8.2662400
C	0.2444500	0.1962300	2.3991500
F	0.6994500	-0.9392500	1.8578300
F	-0.7355800	0.6493000	1.6173600
F	-0.2877800	-0.1073600	3.5933200

LDA

E(SCF)	-1352.1749889		
C	1.9879300	1.5540500	1.3302600
C	1.3286700	1.3354000	2.6718400
C	2.3626000	0.8542600	3.6792500
C	1.9536900	2.9942800	7.8740700
C	1.0821900	3.6345000	6.7834900
C	-0.1233400	2.7398500	6.5350900
O	0.7605100	2.5154500	3.0815400
O	2.6284600	1.4385700	4.7083300
O	2.9809100	-0.2613400	3.3216200
O	1.8172500	3.7926500	5.6355100
O	-0.3797900	2.2309000	5.4644300
O	-0.9006100	2.5808600	7.5959000
H	2.7444800	2.3451100	1.4307500
H	2.4569400	0.6339000	0.9575900
H	1.2182800	1.8962500	0.6233600

F	2.2938000	1.7451500	7.5276800
F	1.3408200	2.9330700	9.0602800
F	3.0738600	3.6940900	8.0330600
H	0.3794200	2.4345200	4.0052600
H	3.6191100	-0.4736300	4.0390800
H	2.0777600	2.9067500	5.2451900
H	-1.6387000	1.9923200	7.3202400
C	0.6196700	4.9932400	7.2548300
H	0.0199800	5.4598000	6.4605200
H	1.5095500	5.6150300	7.4299100
H	0.0266700	4.9193100	8.1759400
C	0.2430100	0.2585700	2.5285400
F	0.7061900	-0.8804000	2.0044600
F	-0.7350800	0.6979300	1.7410800
F	-0.2890300	-0.0312000	3.7239300

PBE

E(SCF)	-1360.4568597		
C	1.9640000	1.5390500	1.1885400
C	1.3316400	1.2463600	2.5531000
C	2.4164700	0.7951000	3.5615300
C	1.9186900	3.0230800	8.0542200
C	1.0748500	3.6884500	6.9215900
C	-0.1748400	2.8179600	6.6423600
O	0.7111100	2.4187000	2.9931900
O	2.6370600	1.3480700	4.6241200
O	3.1280900	-0.2683700	3.1381500
O	1.8564200	3.8073200	5.7691500
O	-0.3965100	2.2563000	5.5845600
O	-1.0265200	2.7584200	7.6852900
H	2.7016000	2.3420700	1.3053700
H	2.4509100	0.6517700	0.7715500
H	1.1778400	1.8856100	0.5075000
F	2.2256600	1.7385300	7.7307600
F	1.2782800	2.9993700	9.2488500
F	3.0797500	3.6892000	8.2301500
H	0.3914400	2.3172800	3.9212200
H	3.7763200	-0.4633900	3.8463400
H	2.0526200	2.9188700	5.3872300
H	-1.7701700	2.1884400	7.3991400
C	0.6549800	5.0994600	7.3462300
H	0.0743400	5.5549400	6.5351000
H	1.5591100	5.6987600	7.5054500

H	0.0553400	5.0828900	8.2618600
C	0.2638500	0.1162000	2.4110500
F	0.7601200	-1.0157000	1.8539500
F	-0.7622900	0.5317600	1.6383600
F	-0.2449300	-0.2172500	3.6271400

MP2

E(SCF)	-1355.1630228		
C	1.9871580	1.5255338	1.2267798
C	1.3334827	1.2578926	2.5727958
C	2.3795301	0.7942645	3.5892179
C	1.9374088	3.0347331	7.9999006
C	1.0731818	3.6782360	6.9011650
C	-0.1417935	2.7873639	6.6319776
O	0.7400096	2.4435530	2.9972485
O	2.5833835	1.3398203	4.6521169
O	3.0748285	-0.2715922	3.1734827
O	1.8325636	3.8221049	5.7432299
O	-0.3485923	2.2185629	5.5819111
O	-0.9787286	2.7169769	7.6745296
H	2.7429073	2.2961022	1.3561360
H	2.4453253	0.6287588	0.8227249
H	1.2276403	1.8954469	0.5435111
F	2.2617531	1.7765329	7.6620212
F	1.3166618	2.9897197	9.1838149
F	3.0698865	3.7187428	8.1630911
H	0.4180573	2.3425385	3.9116883
H	3.7012349	-0.4772665	3.8854411
H	2.0324774	2.9447782	5.3685427
H	-1.7034675	2.1342301	7.3975221
C	0.6258081	5.0648992	7.3344203
H	0.0202289	5.4966394	6.5416143
H	1.5085679	5.6830904	7.4727398
H	0.0508669	5.0272377	8.2538797
C	0.2533795	0.1712399	2.4286996
F	0.7275208	-0.9591060	1.8934308
F	-0.7400194	0.6012036	1.6506894
F	-0.2660450	-0.1329984	3.6287215

BP86

E(SCF)	-1361.8592125		
C	1.9369600	1.5615600	1.1715400
C	1.3215300	1.2271000	2.5373200
C	2.4251400	0.7900400	3.5348900

C	1.8951600	3.0244000	8.1062800
C	1.0827200	3.6898000	6.9472500
C	-0.1814900	2.8392600	6.6600400
O	0.6701100	2.3761500	3.0012700
O	2.6291400	1.3252600	4.6104700
O	3.1734500	-0.2397800	3.0853200
O	1.8875600	3.7709000	5.8046400
O	-0.3916600	2.2544600	5.6118100
O	-1.0599100	2.8258900	7.6851200
H	2.6567500	2.3794500	1.2984300
H	2.4415200	0.6944100	0.7331000
H	1.1376600	1.9028600	0.5029500
F	2.1809100	1.7267200	7.8091500
F	1.2342400	3.0330700	9.2923200
F	3.0687100	3.6691700	8.2924000
H	0.3802500	2.2639500	3.9391100
H	3.8304200	-0.4307800	3.7878500
H	2.0516100	2.8743300	5.4233300
H	-1.8107300	2.2643700	7.3977600
C	0.6874100	5.1201500	7.3394000
H	0.1259200	5.5715300	6.5122700
H	1.6020700	5.7038600	7.4976700
H	0.0765800	5.1352300	8.2479200
C	0.2816500	0.0689000	2.3843400
F	0.8049700	-1.0430000	1.8069400
F	-0.7618000	0.4673200	1.6227100
F	-0.2116300	-0.2973400	3.5994400

PW91

E(SCF)	-1361.4705773		
C	1.9635400	1.5415700	1.1970300
C	1.3306500	1.2509500	2.5607000
C	2.4140700	0.8008700	3.5688000
C	1.9191000	3.0192300	8.0448000
C	1.0758900	3.6842700	6.9137600
C	-0.1721700	2.8144000	6.6338700
O	0.7110800	2.4229800	2.9990200
O	2.6379600	1.3572600	4.6275200
O	3.1211800	-0.2656600	3.1501300
O	1.8566500	3.8046500	5.7624300
O	-0.3960000	2.2583600	5.5749500
O	-1.0205100	2.7485000	7.6772900
H	2.6989300	2.3443200	1.3133200
H	2.4507900	0.6552900	0.7828000

H	1.1786300	1.8856700	0.5160900
F	2.2237700	1.7349000	7.7224100
F	1.2802200	2.9973300	9.2392000
F	3.0802000	3.6835100	8.2190400
H	0.3883900	2.3246100	3.9259000
H	3.7697100	-0.4609900	3.8564800
H	2.0565000	2.9181600	5.3788900
H	-1.7643200	2.1799500	7.3923600
C	0.6550100	5.0935800	7.3396000
H	0.0765500	5.5489500	6.5292100
H	1.5574500	5.6917600	7.5006900
H	0.0549400	5.0752700	8.2528800
C	0.2637000	0.1221600	2.4193000
F	0.7588500	-1.0083100	1.8606500
F	-0.7626500	0.5382100	1.6490500
F	-0.2429000	-0.2125000	3.6348800

Table S6 Cartesian coordinates and SCF energies of Dimer **B-RS** at level of theory given in header

MP2

E(SCF)	-1355.1625754		
C	1.0180027	1.6996086	1.6411302
C	1.1259908	0.6058547	2.7169177
C	2.4521578	0.8091525	3.4533851
C	1.3249810	2.7357203	8.1076049
C	1.2185220	3.8307482	7.0329633
C	-0.1071441	3.6289844	6.2951702
O	0.0613758	0.7388419	3.6084229
O	2.5503882	1.4201574	4.4941526
O	3.4929224	0.2378940	2.8346474
O	2.2838077	3.6981633	6.1421955
O	-0.2049027	3.0187753	5.2538865
O	-1.1480297	4.2006002	6.9133670
F	1.0430754	2.9161573	2.2028947
F	2.0283948	1.6369484	0.7626447
F	-0.1225583	1.5871925	0.9607040
F	1.2998470	1.5198184	7.5444491
F	0.3137814	2.7978890	8.9852018
F	2.4649515	2.8468126	8.7892350
H	0.1929452	1.5343672	4.1505045
H	4.2732697	0.4488315	3.3716539
H	2.1522762	2.9033094	5.5991220
H	-1.9280553	3.9906062	6.3755224
C	1.3126870	5.2023326	7.6740472
H	1.1838427	5.9597525	6.9057167
H	2.3018979	5.3098526	8.1092837
H	0.5551624	5.3353486	8.4394917
C	1.0320746	-0.7665097	2.0774611
H	1.7890698	-0.8999742	1.3115712
H	0.0425796	-0.8750682	1.6431277
H	1.1619367	-1.5229854	2.8465515

PW91

E(SCF)	-1361.4684210		
C	1.0270100	1.7018100	1.6057800
C	1.1327100	0.6075000	2.7117600
C	2.4794800	0.8099500	3.4441900
C	1.3171400	2.7346000	8.1436300
C	1.2116700	3.8291100	7.0378300
C	-0.1350300	3.6268900	6.3051900

O	0.0693100	0.7577200	3.6090400
O	2.5912700	1.4012500	4.4999700
O	3.5260800	0.2542800	2.8036400
O	2.2751600	3.6789700	6.1406500
O	-0.2467400	3.0357400	5.2493200
O	-1.1816600	4.1826000	6.9456700
F	1.0797100	2.9424600	2.1512500
F	2.0305300	1.6138400	0.6962500
F	-0.1403600	1.5979000	0.9381500
F	1.2644300	1.4940500	7.5979200
F	0.3135000	2.8224700	9.0530300
F	2.4844200	2.8383000	8.8114300
H	0.1905000	1.5682900	4.1496300
H	4.3187400	0.4617100	3.3389300
H	2.1539800	2.8685100	5.5999000
H	-1.9742600	3.9753200	6.4102400
C	1.3203900	5.2164700	7.6677600
H	1.2169000	5.9739200	6.8843700
H	2.3110700	5.3158400	8.1215800
H	0.5498400	5.3750700	8.4264300
C	1.0240200	-0.7799800	2.0821000
H	1.7944900	-0.9386600	1.3233600
H	0.0332900	-0.8795000	1.6284000
H	1.1276600	-1.5372800	2.8656100

M05-2X

E(SCF) -1361.7691122

C	1.0127500	1.6883300	1.6458600
C	1.1160200	0.5914800	2.7112000
C	2.4383200	0.7984400	3.4532100
C	1.3312600	2.7478900	8.1033700
C	1.2283700	3.8451500	7.0384300
C	-0.0937900	3.6386300	6.2960500
O	0.0519100	0.7292200	3.5943200
O	2.5253800	1.4096200	4.4834800
O	3.4834000	0.2345200	2.8527200
O	2.2926600	3.7076100	6.1554900
O	-0.1807200	3.0277600	5.2655900
O	-1.1389100	4.2025600	6.8964600
F	1.0168100	2.9004300	2.2152300
F	2.0366500	1.6431100	0.7810200
F	-0.1160500	1.5677400	0.9475900
F	1.3271800	1.5360000	7.5335500

F	0.3071600	2.7929000	8.9679900
F	2.4599100	2.8680600	8.8019600
H	0.1710400	1.5117900	4.1544500
H	4.2692500	0.4426700	3.3765800
H	2.1735700	2.9252500	5.5950500
H	-1.9246800	3.9947000	6.3723600
C	1.3106700	5.2113200	7.6926300
H	1.1764600	5.9729100	6.9313600
H	2.2983800	5.3168600	8.1280400
H	0.5513700	5.3262500	8.4576200
C	1.0337600	-0.7749500	2.0575400
H	1.7929300	-0.8900700	1.2924500
H	0.0459800	-0.8807800	1.6223600
H	1.1682100	-1.5362300	2.8190700

BP86

E(SCF)	-1361.8575380		
C	1.0405200	1.6728100	1.5059800
C	1.1312500	0.6114000	2.6511200
C	2.4736500	0.8249700	3.3950600
C	1.3036700	2.7636100	8.2434200
C	1.2131200	3.8252200	7.0984600
C	-0.1292300	3.6118600	6.3543500
O	0.0573000	0.7998100	3.5343800
O	2.5710400	1.4105700	4.4573400
O	3.5330100	0.2829000	2.7562500
O	2.2871400	3.6369000	6.2152600
O	-0.2265400	3.0264100	5.2919700
O	-1.1886000	4.1539300	6.9931200
F	1.1146400	2.9331300	2.0098600
F	2.0400200	1.5400100	0.5934700
F	-0.1332200	1.5652700	0.8440200
F	1.2295500	1.5033800	7.7393000
F	0.3040800	2.8962900	9.1558400
F	2.4773500	2.8709700	8.9055200
H	0.2096600	1.5952100	4.0923700
H	4.3212700	0.4948600	3.2997700
H	2.1347900	2.8416100	5.6571200
H	-1.9768300	3.9421000	6.4494900
C	1.3264900	5.2363800	7.6834100
H	1.2336100	5.9687400	6.8724100
H	2.3163200	5.3462500	8.1415700
H	0.5506200	5.4261400	8.4323000

C	1.0179100	-0.7998700	2.0664300
H	1.7937200	-0.9897200	1.3175000
H	0.0280400	-0.9098800	1.6083800
H	1.1109000	-1.5320800	2.8775600

B3LYP

E(SCF)	-1361.8565703		
C	1.0403900	1.6703000	1.5124000
C	1.1303800	0.6149000	2.6496800
C	2.4652300	0.8252100	3.3970600
C	1.3038800	2.7661900	8.2370400
C	1.2139800	3.8217200	7.0998800
C	-0.1208300	3.6115300	6.3524000
O	0.0598000	0.8032600	3.5234700
O	2.5534200	1.3991900	4.4526600
O	3.5194800	0.2967300	2.7643900
O	2.2846000	3.6334400	6.2261200
O	-0.2089900	3.0376700	5.2967400
O	-1.1751000	4.1399900	6.9850700
F	1.1052000	2.9186300	2.0135800
F	2.0370200	1.5440800	0.6155700
F	-0.1174200	1.5590300	0.8487900
F	1.2390700	1.5179100	7.7357000
F	0.3072000	2.8923200	9.1338200
F	2.4616500	2.8773500	8.9007300
H	0.1928200	1.5892000	4.0784500
H	4.3074500	0.4956500	3.2936400
H	2.1515900	2.8475600	5.6710400
H	-1.9630500	3.9411500	6.4557500
C	1.3242800	5.2303400	7.6804600
H	1.2304100	5.9548300	6.8740100
H	2.3063400	5.3430900	8.1335600
H	0.5545400	5.4198600	8.4230200
C	1.0200800	-0.7937900	2.0692700
H	1.7897900	-0.9833800	1.3266900
H	0.0380100	-0.9066200	1.6162300
H	1.1140100	-1.5181800	2.8758000

PBE

E(SCF)	-1360.4548056		
C	1.0293500	1.6928000	1.5825600
C	1.1314400	0.6023800	2.6951700
C	2.4771400	0.8071300	3.4316800

C	1.3148500	2.7436400	8.1668600
C	1.2129300	3.8342400	7.0544100
C	-0.1327000	3.6296800	6.3177300
O	0.0645400	0.7584500	3.5892100
O	2.5838800	1.3956800	4.4909000
O	3.5279000	0.2572700	2.7900700
O	2.2799100	3.6782400	6.1604500
O	-0.2393800	3.0412600	5.2584300
O	-1.1835000	4.1795400	6.9593000
F	1.0846000	2.9367600	2.1228700
F	2.0334700	1.5984300	0.6730600
F	-0.1389800	1.5884600	0.9144700
F	1.2595800	1.4997700	7.6263600
F	0.3106300	2.8379400	9.0762700
F	2.4831100	2.8478100	8.8351000
H	0.1959000	1.5646700	4.1347500
H	4.3184500	0.4668300	3.3295600
H	2.1485600	2.8721100	5.6147700
H	-1.9740000	3.9701000	6.4196900
C	1.3211400	5.2255600	7.6782800
H	1.2197700	5.9807300	6.8899800
H	2.3123400	5.3270700	8.1347500
H	0.5479300	5.3886100	8.4357900
C	1.0232500	-0.7890500	2.0715100
H	1.7964000	-0.9521600	1.3139600
H	0.0320200	-0.8906800	1.6151500
H	1.1247400	-1.5440900	2.8599200

LDA

E(SCF)	-1352.1713075		
C	0.6658100	1.4508600	1.7611000
C	1.1902100	0.6984600	2.9929200
C	2.5850300	1.2272700	3.2935300
C	0.9509200	2.3966600	7.6872300
C	1.2477900	3.7060500	6.9428400
C	0.0873000	3.9215900	5.9802000
O	0.3457300	0.9225500	4.0529500
O	2.8453600	1.9609500	4.2200500
O	3.5097600	0.7999600	2.4438200
O	2.4292800	3.5845600	6.2461600
O	0.0334900	3.4231300	4.8753500
O	-0.8616700	4.7199900	6.4439600
F	0.6259200	2.7666600	2.0049200
F	1.4291700	1.2601000	0.6794700

F	-0.5683000	1.0522800	1.4644000
F	0.9484600	1.3646000	6.8407800
F	-0.2477900	2.4374400	8.2886100
F	1.8701000	2.1605700	8.6191200
H	0.3726600	1.8787400	4.3372000
H	4.3578200	1.2159300	2.7171500
H	2.3609400	2.9229200	5.5039100
H	-1.5576100	4.7630100	5.7496200
C	1.3808200	4.8232800	7.9416700
H	1.5526400	5.7684300	7.4088100
H	2.2500100	4.6126100	8.5797800
H	0.4791800	4.9185200	8.5612100
C	1.2233900	-0.7795900	2.6965800
H	1.8711300	-1.0018200	1.8384500
H	0.1965500	-1.1117400	2.4879500
H	1.5911300	-1.3148000	3.5832800