

Monomer, H/H:

-171.142681310 Hartrees (B3LYP/6-311++G**)

C	0.23631	-0.34589	-0.34315
H	0.66378	-1.31584	-0.05656
H	0.32664	-0.23665	-1.42997
N	-1.12424	-0.30472	0.15956
H	-1.58392	-1.20612	0.11264
H	-1.69361	0.38557	-0.31729
O	0.99304	0.72707	0.18771
H	0.79458	0.76487	1.13150

Monomer, F/F:

-369.712720863 Hartrees (B3LYP/6-311++G**)

C	0.00894	-0.01921	-0.01166
N	0.46248	1.18784	-0.59101
O	0.60364	-1.12311	-0.54556
H	0.11119	1.99561	-0.08953
H	0.20333	1.24029	-1.56963
H	1.55185	-0.95046	-0.59369
F	-1.34047	-0.23183	-0.14010
F	0.23086	0.06514	1.34280

Monomer, CH₃/CH₃:

-249.802315577 Hartrees (B3LYP/6-311++G**)

C	0.01120	-0.00951	-0.00830
N	0.73830	-0.59332	1.12216
O	0.69326	-0.41272	-1.19931
C	-1.42003	-0.53164	-0.16916
H	-1.40860	-1.61947	-0.27372
H	-1.88634	-0.11009	-1.06275
H	-2.02582	-0.26637	0.70097
C	0.03984	1.51677	0.13240
H	0.45202	-0.18719	2.00660
H	0.58544	-1.59649	1.17004
H	1.63629	-0.31002	-1.02092
H	1.07077	1.86613	0.23094
H	-0.40193	1.97697	-0.75279
H	-0.52210	1.84781	1.01129

Monomer, CF₃/CF₃:

-845.432136465 Hartrees (B3LYP/6-311++G**)

C	0.52859	-0.33899	-0.01947
N	1.24034	-0.88125	1.10662
O	1.17904	-0.65393	-1.21452
C	-0.90528	-0.94244	-0.18319
C	0.48290	1.21598	0.15858
H	0.89143	-0.54677	1.99783
H	1.22422	-1.89524	1.08960
H	2.12464	-0.51471	-1.07113
F	1.71945	1.71597	-0.02047
F	-0.32945	1.80533	-0.72425
F	0.07934	1.56780	1.39761
F	-0.82072	-2.28876	-0.15765
F	-1.51131	-0.59207	-1.31878
F	-1.69199	-0.56941	0.84776

Monomer, F/H:

-270.429428155 Hartrees (B3LYP/6-311++G**)

C	0.04353	0.04678	-0.35461
F	0.61926	-1.17297	0.02738
H	0.14003	0.08710	-1.44354
N	-1.28778	0.02920	0.18284
H	-1.76457	-0.83852	-0.03519
H	-1.83148	0.81124	-0.16532
O	0.75916	1.10605	0.14441
H	0.56272	1.16344	1.09012

Monomer, H/CH₃:

-210.473738307 Hartrees (B3LYP/6-311++G**)

C	0.13234	-0.02578	0.33203
H	0.48413	-0.05347	1.37339
N	0.71890	1.16778	-0.26452
H	0.69389	1.95991	0.36774
H	0.24571	1.42477	-1.12622
O	0.60645	-1.16888	-0.36950
H	1.54410	-1.01716	-0.53729
C	-1.38993	-0.10222	0.30753
H	-1.73423	-1.04113	0.74722
H	-1.82341	0.72822	0.87050
H	-1.74864	-0.05654	-0.72500

Monomer, H/CF₃:

-508.294418452 Hartrees (B3LYP/6-311++G**)

C	0.01093	-0.93722	-0.20613
H	0.03339	-1.22077	-1.26662
N	-1.16813	-1.51097	0.38892
H	-1.97420	-1.47643	-0.22332
H	-1.39626	-1.08253	1.28051
O	1.16864	-1.35939	0.47192
H	1.02677	-2.28465	0.70426
C	0.04283	0.60297	-0.17498
F	1.17421	1.10512	-0.69250
F	-0.09406	1.08486	1.07684
F	-0.98954	1.09022	-0.90722

Monomer, F/CH₃:

-309.761358313 Hartrees (B3LYP/6-311++G**)

C	-0.01537	-0.02163	-0.02228
F	-0.33547	1.35394	0.04835
N	-0.67747	-0.59821	1.12546
O	-0.54631	-0.55610	-1.17863
H	-0.47181	-0.07307	1.96815
H	-0.39816	-1.56451	1.25716
H	-1.50313	-0.60876	-1.04959
C	1.49912	-0.12196	-0.09619
H	1.79994	-1.17104	-0.12487
H	1.85752	0.37184	-1.00032
H	1.94511	0.35791	0.77589

Monomer, CF₃/CH₃

-547.623950221 Hartrees (B3LYP/6-311++G**)

C	0.02782	-0.77392	-0.04231
N	-1.10977	-1.37347	0.62277
H	-1.95216	-1.34188	0.06093
H	-1.29190	-0.94333	1.52406
O	1.20976	-1.14484	0.64602
H	1.06237	-2.04215	0.96820
C	0.00394	0.77545	0.06001
F	1.09933	1.34969	-0.46436
F	-0.10196	1.18566	1.34074
F	-1.06965	1.27473	-0.60306
C	0.07503	-1.20589	-1.50919
H	0.97391	-0.81134	-1.98226
H	0.10729	-2.29611	-1.54718
H	-0.79954	-0.85681	-2.06216

Dimer H/H, C:

-342.304649399 Hartrees (B3LYP/6-311++G**)

C	1.95881	0.17804	-0.35221
N	1.48858	-1.08317	0.25761
O	1.32609	1.27298	0.23757
H	1.75165	0.10435	-1.42889
H	3.03512	0.33359	-0.21774
H	1.91348	-1.88542	-0.20262
H	1.76646	-1.11178	1.23572
H	0.36505	1.24238	0.01889
C	-1.95881	-0.17804	0.35221
N	-1.48858	1.08317	-0.25761
O	-1.32609	-1.27298	-0.23757
H	-1.75165	-0.10435	1.42889
H	-3.03512	-0.33359	0.21774
H	-1.91348	1.88542	0.20262
H	-1.76646	1.11178	-1.23572
H	-0.36505	-1.24238	-0.01889

Dimer H/H, B:

-342.303779339 Hartrees (B3LYP/6-311++G**)

C	0.32835	1.91060	-0.43271
H	0.36222	1.59422	-1.48546
H	0.51783	2.98933	-0.39426
N	-1.01042	1.55002	0.07626
H	-1.73890	1.93801	-0.51883
H	-1.13659	1.94229	1.00652
O	1.32531	1.31058	0.33682
H	1.24311	0.33198	0.25851
C	-0.32835	-1.92047	-0.38653
H	-0.36222	-1.62957	-1.44660
H	-0.51783	-2.99796	-0.32208
N	1.01042	-1.54773	0.11360
H	1.73890	-1.94996	-0.47196
H	1.13659	-1.91746	1.05305
O	-1.32531	-1.30208	0.36832
H	-1.24311	-0.32565	0.26644

Dimer F/F, C:

-739.447422529 Hartrees (B3LYP/6-311++G**)

C	1.93259	0.20393	-0.40310
N	1.43540	-1.01703	0.17713
O	1.35930	1.30682	0.09423
H	1.90749	-1.81648	-0.23849
H	1.62431	-1.01117	1.17661
H	0.37246	1.23111	0.01930
F	3.28413	0.33008	-0.23711
F	1.74238	0.08708	-1.76686
C	-1.93259	-0.20393	0.40310
N	-1.43540	1.01703	-0.17713
O	-1.35930	-1.30682	-0.09423
H	-1.90749	1.81648	0.23849
H	-1.62431	1.01117	-1.17661
H	-0.37246	-1.23111	-0.01930
F	-3.28413	-0.33008	0.23711
F	-1.74238	-0.08708	1.76686

Dimer F/F, B:

-739.445982820

C	0.33062	1.92482	0.01308
N	-0.95159	1.51424	0.53012
H	-1.69534	1.98076	0.01631
H	-1.01488	1.78720	1.50787
O	1.36546	1.28442	0.57534
H	1.23243	0.30391	0.50669
F	0.53692	3.26662	0.19068
F	0.27709	1.73790	-1.34878
C	-0.33062	-1.92482	0.01308
N	0.95159	-1.51424	0.53012
H	1.69534	-1.98076	0.01631
H	1.01488	-1.78720	1.50787
O	-1.36546	-1.28442	0.57534
H	-1.23243	-0.30391	0.50669
F	-0.53692	-3.26662	0.19068
F	-0.27709	-1.73790	-1.34878

Dimer CH₃/CH₃, C

-499.622380925 Hartrees (B3LYP/6-311++G**)

C	-2.09633	0.10625	-0.03027
N	-1.37811	-0.53927	1.10126
O	-1.41581	-0.23311	-1.21873
C	-3.52322	-0.42572	-0.19422
H	-3.49818	-1.50261	-0.37999
H	-4.01118	0.05266	-1.04642
H	-4.11830	-0.23492	0.70296
C	-2.09244	1.62193	0.21148
H	-1.80046	-0.28127	1.99022
H	-1.46598	-1.54948	1.01332
H	-0.48190	0.07568	-1.16526
H	-1.06992	1.98496	0.33347
H	-2.54773	2.12876	-0.64118
H	-2.65816	1.88490	1.11088
C	2.09633	-0.10625	0.03027
N	1.37811	0.53927	-1.10126
O	1.41581	0.23311	1.21873
C	3.52322	0.42572	0.19422
H	3.49818	1.50261	0.37999
H	4.01118	-0.05266	1.04642
H	4.11830	0.23492	-0.70296
C	2.09244	-1.62193	-0.21148
H	1.80046	0.28127	-1.99022
H	1.46598	1.54948	-1.01332
H	0.48190	-0.07568	1.16526
H	1.06992	-1.98496	-0.33347
H	2.54773	-2.12876	0.64118
H	2.65816	-1.88490	-1.11088

Dimer CH₃/CH₃, B:

-499.620753059 Hartrees (B3LYP/6-311++G**)

C	0.38424	2.12272	0.01163
N	-0.94281	1.57087	0.38418
H	-1.68821	2.06680	-0.09815
H	-1.09017	1.70954	1.38196
O	1.37234	1.31145	0.61088
H	1.20016	0.36896	0.39347
C	-0.38424	-2.12272	0.01163
N	0.94281	-1.57087	0.38418
H	1.68821	-2.06680	-0.09815
H	1.09017	-1.70954	1.38196
O	-1.37234	-1.31145	0.61088
H	-1.20016	-0.36896	0.39347
C	-0.60776	-3.53491	0.56244
H	-1.60615	-3.89190	0.29972
H	0.13116	-4.23358	0.16072
H	-0.52871	-3.52377	1.65245
C	-0.49875	-2.10426	-1.51867
H	-0.36914	-1.08854	-1.89758
H	0.25373	-2.74685	-1.98672
H	-1.48730	-2.45961	-1.81451
C	0.60776	3.53491	0.56244
H	1.60615	3.89190	0.29972
H	-0.13116	4.23358	0.16072
H	0.52871	3.52377	1.65245
C	0.49875	2.10426	-1.51867
H	0.36914	1.08854	-1.89758
H	-0.25373	2.74685	-1.98672
H	1.48730	2.45961	-1.81451

Dimer CF₃/CF₃, C:

-1690.88319148 Hartrees (B3LYP/6-311++G**)

C	-2.08405	0.18418	-0.08681
N	-1.38154	-0.41603	1.04505
O	-1.43177	-0.06814	-1.27556
C	-3.51117	-0.43311	-0.25984
C	-2.16221	1.72626	0.18227
H	-1.83388	-0.19628	1.92929
H	-1.37567	-1.42692	0.92956
H	-0.45966	0.07572	-1.17022
F	-0.92914	2.26179	0.06284
F	-2.96308	2.35252	-0.68279
F	-2.59568	1.99777	1.43049
F	-3.40463	-1.77568	-0.32066
F	-4.13668	-0.01866	-1.36057
F	-4.28881	-0.14067	0.80538
C	2.08405	-0.18418	0.08681
N	1.38154	0.41603	-1.04505
O	1.43177	0.06814	1.27556
C	3.51117	0.43311	0.25984
C	2.16221	-1.72626	-0.18227
H	1.83388	0.19628	-1.92929
H	1.37567	1.42692	-0.92956
H	0.45966	-0.07572	1.17022
F	0.92914	-2.26179	-0.06284
F	2.96308	-2.35252	0.68279
F	2.59568	-1.99777	-1.43049
F	3.40463	1.77568	0.32066
F	4.13668	0.01866	1.36057
F	4.28881	0.14067	-0.80538

Dimer CF₃/CF₃, B:

-1690.87946517 Hartrees (B3LYP/6-311++G**)

C	-0.00154	2.17103	-0.25518
N	1.19043	1.37196	-0.52031
H	2.01076	1.75254	-0.05578
H	1.36982	1.36222	-1.52173
O	-1.14992	1.51418	-0.65771
H	-1.10365	0.56511	-0.40271
C	0.00154	-2.17103	-0.25518
N	-1.19043	-1.37196	-0.52031
H	-2.01076	-1.75254	-0.05578
H	-1.36982	-1.36222	-1.52173
O	1.14992	-1.51418	-0.65771
H	1.10365	-0.56511	-0.40271
C	-0.01635	-3.50293	-1.07643
F	1.12824	-4.18032	-1.01493
F	-1.01252	-4.30976	-0.65580
F	-0.25731	-3.21407	-2.37435
C	0.05367	-2.46007	1.28484
F	0.38355	-1.33651	1.93905
F	-1.14520	-2.86858	1.75795
F	0.95774	-3.39641	1.58861
C	0.01635	3.50293	-1.07643
F	-1.12824	4.18032	-1.01493
F	1.01252	4.30976	-0.65580
F	0.25731	3.21407	-2.37435
C	-0.05367	2.46007	1.28484
F	-0.38355	1.33651	1.93905
F	1.14520	2.86858	1.75795
F	-0.95774	3.39641	1.58861

Dimer F/H (R/R), C-1:

-540.877106930 Hartrees (B3LYP/6-311++G**)

C	-1.82012	-0.53748	-0.00429
F	-3.17875	-0.20711	0.01495
N	-1.16116	0.07443	-1.13082
O	-1.30557	-0.08954	1.18278
H	-1.78886	-1.62830	-0.11762
H	-1.24537	1.08714	-1.05908
H	-1.58878	-0.22316	-2.00394
H	-0.32396	-0.18987	1.17370
C	2.19699	0.10282	-0.05380
F	2.02706	1.49687	0.03550
N	1.54319	-0.42481	1.13812
O	1.65327	-0.39444	-1.19005
H	3.27731	-0.06035	-0.09083
H	1.92307	0.01793	1.97127
H	1.72308	-1.42353	1.20440
H	0.67173	-0.25524	-1.17636

Dimer F/H (R/R), B-1:

-540.874856712 Hartrees (B3LYP/6-311++G**)

C	0.33151	1.91168	-0.36462
H	0.29870	1.71688	-1.44373
F	0.55736	3.28318	-0.23879
N	-0.93532	1.54763	0.22146
H	-1.69877	2.03679	-0.23884
H	-0.93314	1.81265	1.20499
O	1.37640	1.29803	0.27578
H	1.25481	0.32034	0.23677
C	-0.33151	-1.91992	-0.31843
H	-0.29870	-1.75118	-1.40193
F	-0.55736	-3.28798	-0.15958
N	0.93532	-1.54184	0.25870
H	1.69877	-2.04196	-0.18967
H	0.93314	-1.78308	1.24833
O	-1.37640	-1.29101	0.30699
H	-1.25481	-0.31454	0.24443

Dimer F/H (R/R), B-2:

-540.877266764 Hartrees (B3LYP/6-311++G**)

C	0.32518	1.99655	0.04839
H	0.51133	3.06595	0.18235
N	-0.95242	1.53242	0.57876
H	-1.71854	1.98190	0.08372
H	-1.02071	1.78528	1.56136
O	1.36899	1.31769	0.58239
H	1.20216	0.34305	0.52903
C	-0.32518	-1.99480	0.09650
H	-0.51133	-3.06066	0.25621
N	0.95242	-1.51803	0.61553
H	1.71854	-1.97931	0.13147
H	1.02071	-1.74713	1.60394
O	-1.36899	-1.30326	0.61398
H	-1.20216	-0.33020	0.53715
F	-0.22826	-1.83295	-1.29396
F	0.22826	1.80122	-1.33777

Dimer F/H (R/S), C-2:

-540.875398689 Hartrees (B3LYP/6-311++G**)

C	1.95671	0.05011	-0.30371
F	3.32953	0.11321	-0.05948
N	1.39823	-1.15978	0.25089
O	1.41709	1.16475	0.28373
H	1.84756	0.02911	-1.39450
H	1.57717	-1.17724	1.25335
H	1.83101	-1.98098	-0.16472
H	0.45574	1.21326	0.06703
C	-1.95671	-0.05011	0.30371
F	-3.32953	-0.11321	0.05948
N	-1.39823	1.15978	-0.25089
O	-1.41709	-1.16475	-0.28373
H	-1.84756	-0.02911	1.39450
H	-1.83101	1.98098	0.16472
H	-1.57717	1.17724	-1.25335
H	-0.45574	-1.21326	-0.06703

Dimer F/H (R/S), C-3:

-540.879610450 Hartrees (B3LYP/6-311++G**)

C	1.97047	0.29300	-0.42360
N	1.50503	-0.87964	0.30243
O	1.29168	1.40754	-0.06771
H	3.04071	0.49605	-0.33121
H	2.03485	-1.70264	0.02777
H	1.63523	-0.73353	1.30033
H	0.31728	1.22961	-0.10211
C	-1.97047	-0.29300	0.42360
N	-1.50503	0.87964	-0.30243
O	-1.29168	-1.40754	0.06771
H	-3.04071	-0.49605	0.33121
H	-2.03485	1.70264	-0.02777
H	-1.63523	0.73353	-1.30033
H	-0.31728	-1.22961	0.10211
F	-1.77045	0.02684	1.78382
F	1.77045	-0.02684	-1.78382

Dimer F/H (R/S), B-3:

-540.877921039 Hartrees (B3LYP/6-311++G**)

C	0.33337	2.10238	-0.17045
H	0.52342	3.17677	-0.23569
N	-0.93169	1.74302	0.45561
H	-1.70493	2.20339	-0.01777
H	-0.92581	2.04879	1.42516
O	1.38868	1.51903	0.44341
H	1.25015	0.53768	0.49761
C	-0.23965	-1.64392	-0.15252
H	-0.17673	-1.35671	-1.20774
N	0.99965	-1.30499	0.50671
H	1.78893	-1.74438	0.03960
H	0.96560	-1.63982	1.46774
O	-1.31330	-1.10045	0.50402
H	-1.24009	-0.11790	0.46274
F	-0.43865	-3.02643	-0.13973
F	0.20292	1.66272	-1.50577

Dimer H/CH₃ (R/R), C-1:
-420.965758012 Hartrees (B3LYP/6-311++G**)

C	-1.78946	-0.59527	-0.00913
N	-1.22348	0.09996	-1.18761
O	-1.23242	-0.04926	1.15627
C	-3.30560	-0.48990	0.10877
H	-1.50396	-1.65176	-0.12438
H	-1.56924	-0.31705	-2.04927
H	-1.52791	1.07188	-1.17989
H	-0.26204	-0.21912	1.15645
H	-3.65559	-1.04398	0.98267
H	-3.79648	-0.89383	-0.78094
H	-3.59728	0.55770	0.22902
C	2.24351	0.14296	-0.06131
N	1.61024	-0.53299	1.09557
O	1.63430	-0.30972	-1.24086
C	2.15439	1.65644	0.12356
H	3.29771	-0.14608	-0.15846
H	2.02364	-0.21962	1.97062
H	1.77526	-1.53420	1.02632
H	0.67309	-0.09104	-1.21966
H	2.58119	2.15501	-0.74852
H	2.70917	1.98098	1.00992
H	1.11305	1.96886	0.23585

Dimer H/CH₃ (R/R), B-1:
-420.966204406 Hartrees (B3LYP/6-311++G**)

C	-1.97217	-0.05126	0.33299
H	-1.64464	-0.09216	1.38363
N	-1.38473	1.19091	-0.22011
H	-1.69147	2.00083	0.31436
H	-1.71653	1.31674	-1.17515
O	-1.48729	-1.14918	-0.38947
H	-0.50412	-1.17173	-0.32205
C	-3.49489	-0.09733	0.27902
H	-3.86001	-1.02885	0.71742
H	-3.93176	0.74183	0.82746
H	-3.83066	-0.05423	-0.76123
C	1.97217	0.05126	0.33299
H	1.64464	0.09216	1.38363
N	1.38473	-1.19091	-0.22011
H	1.69147	-2.00083	0.31436
H	1.71653	-1.31674	-1.17515
O	1.48729	1.14918	-0.38947
H	0.50412	1.17173	-0.32205
C	3.49489	0.09733	0.27902
H	3.86001	1.02885	0.71742
H	3.93176	-0.74183	0.82746
H	3.83066	0.05423	-0.76123

Dimer H/CH₃ (R/R), B-2:
-420.962943550 Hartrees (B3LYP/6-311++G**)

C	-2.12739	-0.15033	0.09228
H	-3.15490	-0.53542	0.12275
N	-1.44159	-0.54406	-1.15615
H	-1.83718	-0.06027	-1.95802
H	-1.57064	-1.54108	-1.31087
O	-1.48362	-0.76185	1.18083
H	-0.52391	-0.55339	1.15227

C	2.12739	-0.15033	-0.09228
H	3.15490	-0.53542	-0.12275
N	1.44159	-0.54406	1.15615
H	1.83718	-0.06027	1.95802
H	1.57064	-1.54108	1.31087
O	1.48362	-0.76185	-1.18083
H	0.52391	-0.55339	-1.15227
C	-2.16898	1.37258	0.19960
H	-2.64278	1.65723	1.14058
H	-1.15842	1.78836	0.17886
H	-2.74260	1.81434	-0.62181
C	2.16898	1.37258	-0.19960
H	1.15842	1.78836	-0.17886
H	2.74260	1.81434	0.62181
H	2.64278	1.65723	-1.14058

Dimer H/CH₃ (R/S), C-2:
-420.966851757 Hartrees (B3LYP/6-311++G**)

C	2.00793	0.04869	-0.30528
H	1.79537	0.02787	-1.38487
N	1.38864	-1.17960	0.24582
H	1.61171	-1.24708	1.23744
H	1.77184	-2.00732	-0.20599
O	1.42183	1.16749	0.30130
H	0.46109	1.18834	0.07873
C	3.51384	0.13689	-0.08700
H	3.73387	0.16277	0.98438
H	3.90738	1.05050	-0.53826
H	4.02503	-0.72100	-0.53254
C	-2.00793	-0.04869	0.30528
H	-1.79537	-0.02787	1.38487
N	-1.38864	1.17960	-0.24582
H	-1.77184	2.00732	0.20599
H	-1.61171	1.24708	-1.23744
O	-1.42183	-1.16749	-0.30130
H	-0.46109	-1.18834	-0.07873
C	-3.51384	-0.13689	0.08700
H	-4.02503	0.72100	0.53254
H	-3.90738	-1.05050	0.53826
H	-3.73387	-0.16277	-0.98438

Dimer H/CH₃ (R/S), C-3:

-420.964509433 Hartrees (B3LYP/6-311++G**)

C	2.05468	0.09244	-0.28845
N	1.31603	1.30994	0.11709
O	1.28643	-0.61406	-1.22762
H	2.98090	0.34810	-0.81858
H	1.83062	1.82910	0.82439
H	1.21160	1.92171	-0.68851
H	0.42993	-0.87735	-0.81920
C	2.39951	-0.73009	0.95145
H	2.89841	-1.65240	0.64868
H	3.07137	-0.17941	1.61780
H	1.49394	-0.98271	1.50880
C	-2.05468	-0.09244	0.28845
N	-1.31603	-1.30994	-0.11709
O	-1.28643	0.61406	1.22762
H	-2.98090	-0.34810	0.81858
H	-1.83062	-1.82910	-0.82439
H	-1.21160	-1.92171	0.68851
H	-0.42993	0.87735	0.81920
C	-2.39951	0.73009	-0.95145
H	-2.89841	1.65240	-0.64868
H	-3.07137	0.17941	-1.61780
H	-1.49394	0.98271	-1.50880

Dimer H/CH₃ (R/S), B-3:

-420.965049383 Hartrees (B3LYP/6-311++G**)

C	0.34801	2.21619	-0.17305
H	0.51374	3.28604	0.00805
N	-0.95389	1.77530	0.37666
H	-1.72553	2.22563	-0.10937
H	-1.01065	2.05072	1.35428
O	1.37832	1.56716	0.52240
H	1.25476	0.59179	0.45349
C	-0.28646	-1.76126	-0.08358
H	-0.26272	-1.49784	-1.15283
N	1.01048	-1.30988	0.46776
H	1.78285	-1.75888	-0.01944
H	1.06924	-1.58628	1.44653
O	-1.32447	-1.08953	0.57679
H	-1.20510	-0.11859	0.46564
C	-0.54052	-3.25785	0.05666
H	-1.50217	-3.52074	-0.39005
H	0.24445	-3.83559	-0.43921
H	-0.56842	-3.53307	1.11505
C	0.37971	1.95841	-1.67845
H	0.22155	0.89764	-1.89113
H	-0.39460	2.53310	-2.19706
H	1.35136	2.25422	-2.07787

Dimer H/CF₃ (R/R), C-1:

-1016.60720343 Hartrees (B3LYP/6-311++G**)

C	-1.45454	-0.95185	-0.03945
N	-0.92551	-0.21469	-1.18798
O	-0.95272	-0.44611	1.14946
C	-2.98922	-0.87903	0.05747
F	-3.46620	-1.60283	1.08091
F	-3.53878	-1.37745	-1.08190
F	-3.43279	0.38412	0.19255
H	-1.21582	-2.01483	-0.18942

H	-1.30171	-0.57288	-2.06259
H	-1.17695	0.76872	-1.10986
H	0.02750	-0.54217	1.14631
C	2.54333	-0.21445	-0.14939
N	1.89826	-0.80255	1.03511
O	1.89408	-0.59654	-1.31054
C	2.58025	1.31896	0.01727
F	3.29398	1.88960	-0.96472
F	3.16621	1.65593	1.19605
F	1.35201	1.87008	0.00808
H	3.59067	-0.52016	-0.25922
H	2.33489	-0.47415	1.89353
H	2.02568	-1.81057	0.99815
H	0.92703	-0.38900	-1.25222

Dimer H/CF₃ (R/R), B-1:

-1016.60824819 Hartrees (B3LYP/6-311++G**)

C	-0.00575	1.92388	-0.21185
H	0.06387	1.66175	-1.27738
N	-1.24935	1.34705	0.30612
H	-2.05203	1.64154	-0.24503
H	-1.39403	1.65738	1.26526
O	1.08623	1.49584	0.52496
H	1.17780	0.51812	0.42872
C	-0.00387	3.46285	-0.16163
C	0.00575	-1.92388	-0.21185
H	-0.06387	-1.66175	-1.27738
N	1.24935	-1.34705	0.30612
H	2.05203	-1.64154	-0.24503
H	1.39403	-1.65738	1.26526
O	-1.08623	-1.49584	0.52496
H	-1.17780	-0.51812	0.42872
C	0.00387	-3.46285	-0.16163
F	1.11588	3.98443	-0.68174
F	-0.14349	3.92986	1.09312
F	-1.04966	3.94101	-0.88618
F	-1.11588	-3.98443	-0.68174
F	1.04966	-3.94101	-0.88618
F	0.14349	-3.92986	1.09312

Dimer H/CF₃ (R/R), B-2:

-1016.60297951 Hartrees (B3LYP/6-311++G**)

C	-2.16017	0.95468	0.08277
C	2.16017	0.95468	-0.08277
H	-3.14159	1.43889	0.15193
H	3.14159	1.43889	-0.15193
N	-1.33308	1.16169	1.27672
N	1.33308	1.16169	-1.27672
H	-1.66586	0.60586	2.06037
H	1.66586	0.60586	-2.06037
H	-1.39411	2.13883	1.55016
H	1.39411	2.13883	-1.55016
O	-1.54487	1.47323	-1.04837
O	1.54487	1.47323	1.04837
H	-0.60554	1.18121	-1.08134
H	0.60554	1.18121	1.08134
C	-2.46095	-0.55013	-0.07861
C	2.46095	-0.55013	0.07861
F	-1.36551	-1.26812	-0.37144
F	1.36551	-1.26812	0.37144
F	2.98907	-1.05972	-1.06705
F	-2.98907	-1.05972	1.06705
F	3.35967	-0.75103	1.05585
F	-3.35967	-0.75103	-1.05585

Dimer H/CF₃ (R/S), C-2:

-1016.60928855 Hartrees (B3LYP/6-311++G**)

C	1.94543	-0.00392	0.23074
H	1.80377	-0.01437	1.32009
N	1.36140	1.24056	-0.27908
H	1.55649	1.32673	-1.27452
H	1.75303	2.05377	0.19063
O	1.38813	-1.10588	-0.39810
H	0.44965	-1.20534	-0.10605
C	3.46577	-0.07766	0.00284
F	3.78625	-0.02569	-1.30428
F	4.00098	-1.19145	0.52186
F	4.06801	0.98130	0.60503
C	-1.94543	0.00392	-0.23074
H	-1.80377	0.01437	-1.32009
N	-1.36140	-1.24056	0.27908
H	-1.55649	-1.32673	1.27452
H	-1.75303	-2.05377	-0.19063
O	-1.38813	1.10588	0.39810
H	-0.44965	1.20534	0.10605
C	-3.46577	0.07766	-0.00284
F	-3.78625	0.02569	1.30428
F	-4.00098	1.19145	-0.52186
F	-4.06801	-0.98130	-0.60503

Dimer H/CF₃ (R/S), C-3:

-1016.60660432 Hartrees (B3LYP/6-311++G**)

C	-1.28158	-0.49847	-1.56914
N	-0.85451	-1.47067	-0.55410
O	-0.25985	0.38516	-1.87264
H	-1.58487	-0.96682	-2.51391
H	-1.59547	-2.13638	-0.34849
H	-0.06403	-1.99096	-0.92595
H	0.12959	0.74847	-1.04061
C	2.54111	-0.23096	1.05828
F	3.05440	-1.02599	2.00917

F	3.50301	0.66249	0.71141
F	2.29641	-0.99582	-0.02547
C	1.28158	0.49847	1.56914
N	0.85451	1.47067	0.55410
O	0.25985	-0.38516	1.87264
H	1.58487	0.96682	2.51391
H	1.59547	-2.13638	0.34849
H	0.06403	1.99096	0.92595
H	-0.12959	-0.74847	1.04061
C	-2.54111	0.23096	-1.05828
F	-3.05440	1.02599	-2.00917
F	-3.50301	-0.66249	-0.71141
F	-2.29641	0.99582	0.02547

Dimer H/CF₃ (R/S), B-3:

-1016.60809528 Hartrees (B3LYP/6-311++G**)

C	0.42841	2.56437	0.27004
H	0.62494	3.62810	0.45239
N	-0.89116	2.13234	0.75185
H	-1.63938	2.63305	0.27821
H	-0.95455	2.35405	1.74229
O	1.44252	1.85972	0.89444
H	1.27542	0.88548	0.83925
C	-0.26564	-1.38142	0.35291
H	-0.24035	-1.20567	-0.72972
N	1.03035	-0.97282	0.89798
H	1.79695	-1.41545	0.39724
H	1.09302	-1.24208	1.87783
O	-1.30284	-0.70844	0.98423
H	-1.19913	0.25575	0.81862
C	-0.53500	-2.88534	0.53476
C	0.46809	2.39966	-1.26331
F	-1.70247	-3.26110	-0.00675
F	0.44551	-3.59974	-0.07713
F	-0.53834	-3.24862	1.83255
F	1.60067	2.90091	-1.77414
F	0.38320	1.10659	-1.64555
F	-0.56900	3.05709	-1.84238

Dimer F/CH₃ (R/R), C-1:

-619.541230310 Hartrees (B3LYP/6-311++G**)

C	2.06272	-0.01080	0.02935
F	3.26215	-0.72574	0.24238
N	1.23141	-0.74905	-0.89979
O	1.46011	0.04494	1.26662
H	1.06170	-1.67827	-0.51939
H	1.70293	-0.85730	-1.79353
H	0.49910	0.24365	1.16536
C	-2.06429	0.02839	-0.04197
F	-2.03039	-1.34497	0.31858
N	-1.32685	0.68051	1.04478
O	-1.42363	0.21296	-1.22941
H	-1.74973	0.45104	1.94078
H	-1.37881	1.68896	0.92539
H	-0.48069	-0.07859	-1.13750
C	-3.52556	0.41664	-0.18158
H	-3.60506	1.47569	-0.43497
H	-3.98002	-0.16956	-0.98088
H	-4.05949	0.22657	0.75085
C	2.46076	1.34916	-0.52556
H	1.57163	1.96230	-0.68388
H	3.11083	1.84146	0.19738
H	2.99632	1.24666	-1.47222

Dimer F/CH₃ (R/R), B-1:

-619.537901278 Hartrees (B3LYP/6-311++G**)

C	-2.06411	-0.00656	0.13993
N	-1.41389	-0.65744	-0.97966
H	-1.87399	-0.40924	-1.85119
H	-1.50164	-1.66506	-0.86333
O	-1.42291	-0.32413	1.31813
H	-0.45127	-0.38932	1.17171
F	-3.36769	-0.53385	0.28155
C	-2.22674	1.48919	-0.08405
H	-2.73409	1.91358	0.78187
H	-1.24944	1.96294	-0.19072
H	-2.82134	1.69117	-0.97784
C	2.06411	-0.00656	-0.13993
N	1.41389	-0.65744	0.97966
H	1.87399	-0.40924	1.85119
H	1.50164	-1.66506	0.86333
O	1.42291	-0.32413	-1.31813
H	0.45127	-0.38932	-1.17171
F	3.36769	-0.53385	-0.28155
C	2.22674	1.48919	0.08405
H	2.73409	1.91358	-0.78187
H	1.24944	1.96294	0.19072
H	2.82134	1.69117	0.97784

Dimer F/CH₃ (R/R), B-2:

-619.541500917 Hartrees (B3LYP/6-311++G**)

C	-0.13928	2.04021	-0.02300
N	1.09646	1.42002	-0.51509
H	1.89333	1.78192	0.00257
H	1.22512	1.66064	-1.49473
O	-1.22880	1.43075	-0.56747
H	-1.14799	0.44828	-0.47513
C	-0.24858	3.54329	-0.21684
H	-0.25933	3.78229	-1.28220
H	-1.17803	3.89703	0.23056

F	-0.09148	1.80563	1.37153
C	0.13928	-2.04021	-0.02300
N	-1.09646	-1.42002	-0.51509
H	-1.89333	-1.78192	0.00257
H	-1.22512	-1.66064	-1.49473
O	1.22880	-1.43075	-0.56747
H	1.14799	-0.44828	-0.47513
H	0.59316	4.04849	0.25956
C	0.24858	-3.54329	-0.21684
H	-0.59316	-4.04849	0.25956
H	0.25933	-3.78229	-1.28220
H	1.17803	-3.89703	0.23056
F	0.09148	-1.80563	1.37153

Dimer F/CH₃ (R/S), C-2:

-619.538875537 Hartrees (B3LYP/6-311++G**)

C	1.92976	0.28739	-0.58299
N	1.52258	-0.98493	-0.01529
O	1.33062	1.32216	0.10587
H	1.97748	-1.75642	-0.49650
H	1.81843	-1.00925	0.95829
H	0.35037	1.22959	0.05137
C	1.71307	0.32796	-2.08834
H	2.05143	1.29409	-2.46207
H	2.28119	-0.46201	-2.58458
H	0.65455	0.20091	-2.32174
F	3.30749	0.46730	-0.35991
C	-1.92976	-0.28739	0.58299
N	-1.52258	0.98493	0.01529
O	-1.33062	-1.32216	-0.10587
H	-1.97748	1.75642	0.49650
H	-1.81843	1.00925	-0.95829
H	-0.35037	-1.22959	-0.05137
F	-3.30749	-0.46730	0.35991
C	-1.71307	-0.32796	2.08834
H	-2.28119	0.46201	2.58458
H	-2.05143	-1.29409	2.46207
H	-0.65455	-0.20091	2.32174

Dimer F/CH₃ (R/S), C-3:

-619.544073865 Hartrees (B3LYP/6-311++G**)

C	2.04795	0.02267	-0.13944
N	1.29892	-1.12022	0.38597
O	1.47060	1.18942	0.25236
H	1.73018	-1.99287	0.09283
H	1.30503	-1.08770	1.40227
H	0.49597	1.15565	0.07362
C	3.53278	0.05047	0.17831
H	4.01590	-0.85769	-0.18616
H	3.98910	0.91590	-0.30336
H	3.67867	0.13101	1.25717
F	1.93384	-0.12999	-1.55073
C	-2.04795	-0.02267	0.13944
N	-1.29892	1.12022	-0.38597
O	-1.47060	-1.18942	-0.25236
H	-1.73018	1.99287	-0.09283
H	-1.30503	1.08770	-1.40227
H	-0.49597	-1.15565	-0.07362
C	-3.53278	-0.05047	-0.17831
H	-4.01590	0.85769	0.18616
H	-3.98910	-0.91590	0.30336
H	-3.67867	-0.13101	-1.25717

Dimer F/CH₃ (R/S), B-3:

-619.542226443 Hartrees (B3LYP/6-311++G**)

C	1.99606	-0.03252	-0.03125
N	1.36429	-0.48375	1.21002
H	1.72191	0.04746	1.99975
H	1.58866	-1.46347	1.36353
O	1.47967	-0.69503	-1.10050
H	0.48877	-0.68379	-1.06543
C	-1.99379	-0.01000	0.02493
N	-1.36976	-0.76152	-1.04976
H	-1.73957	-0.47118	-1.95107
H	-1.59519	-1.74601	-0.92217
O	-1.51141	-0.44727	1.24135
H	-0.52711	-0.39812	1.23602
F	-3.36875	-0.32195	0.05733
F	1.64136	1.34681	-0.09375
C	-1.87850	1.49039	-0.19039
H	-0.82937	1.78926	-0.19022
H	-2.33647	1.78367	-1.13806
H	-2.39859	1.99589	0.62318
C	3.51268	-0.09543	-0.07211
H	3.86595	0.31276	-1.01956
H	3.93902	0.48378	0.74852
H	3.84206	-1.13325	0.00760

Dimer CF₃/CH₃ (R/R), C-1:

-1095.26543469 Hartrees (B3LYP/6-311++G**)

C	1.84294	0.42162	-0.00592
N	1.03506	-0.08123	-1.12551
O	1.21308	0.10803	1.20049
C	3.20350	-0.32422	0.05938
F	3.97053	0.08921	1.08128
F	3.90985	-0.11501	-1.08385
F	3.03967	-1.65548	0.17802
H	1.47580	0.11790	-2.01966
H	0.92412	-1.08954	-1.04422
H	0.27133	0.39223	1.16243
C	-2.35291	0.70176	-0.03333
N	-1.54270	0.97766	1.17192
O	-1.61483	1.01401	-1.17324
C	-2.67728	-0.81937	-0.01042
F	-3.48362	-1.16985	-1.02467
F	-3.30363	-1.16769	1.14446
F	-1.56566	-1.57673	-0.09851
H	-2.00630	0.63672	2.01116
H	-1.45850	1.98675	1.26876
H	-0.71789	0.59885	-1.13317
C	-3.65512	1.50320	-0.09334
H	-3.40303	2.56549	-0.09097
H	-4.19927	1.28218	-1.01158
H	-4.29338	1.28484	0.76469
C	2.08391	1.92511	-0.17881
H	1.11875	2.43304	-0.20685
H	2.66108	2.30424	0.66435
H	2.62035	2.14730	-1.10387

Dimer CF₃/CH₃ (R/R), B-1:

-1095.26454114 Hartrees (B3LYP/6-311++G**)

C	0.39815	2.06351	-0.26913
N	-0.89281	1.54900	0.20838
H	-1.66948	2.06446	-0.19663
H	-0.94697	1.64964	1.22002
O	1.43316	1.28951	0.26182
H	1.23131	0.33669	0.12142
C	-0.39815	-2.06351	-0.26913
N	0.89281	-1.54900	0.20838
H	1.66948	-2.06446	-0.19663
H	0.94697	-1.64964	1.22002
O	-1.43316	-1.28951	0.26182
H	-1.23131	-0.33669	0.12142
C	-0.64803	-3.49142	0.28890
C	-0.41378	-2.10043	-1.80047
H	-0.28792	-1.08498	-2.17753
H	0.38543	-2.72667	-2.20224
H	-1.37264	-2.48375	-2.14895
C	0.64803	3.49142	0.28890
C	0.41378	2.10043	-1.80047
H	0.28792	1.08498	-2.17753
H	-0.38543	2.72667	-2.20224
H	1.37264	2.48375	-2.14895
F	-0.59533	-3.51649	1.63521
F	0.31159	-4.34372	-0.15872
F	-1.83429	-3.99428	-0.08594
F	0.59533	3.51649	1.63521
F	1.83429	3.99428	-0.08594
F	-0.31159	4.34372	-0.15872

Dimer CF₃/CH₃ (R/R), B-2:

-1095.26185087 Hartrees (B3LYP/6-311++G**)

C	0.41524	2.16789	0.76014
N	-0.92583	1.57988	0.93595
H	-1.62416	2.08700	0.39824
H	-1.18539	1.66237	1.91600
O	1.38445	1.27308	1.21942
H	1.17445	0.36144	0.91671
C	-0.41524	-2.16789	0.76014
N	0.92583	-1.57988	0.93595
H	1.62416	-2.08700	0.39824
H	1.18539	-1.66237	1.91600
O	-1.38445	-1.27308	1.21942
H	-1.17445	-0.36144	0.91671
C	-0.61357	-3.48398	1.51547
H	-1.63418	-3.84640	1.39293
H	0.08389	-4.24779	1.16680
H	-0.43998	-3.29850	2.57746
C	-0.61206	-2.40617	-0.76422
C	0.61357	3.48398	1.51547
H	1.63418	3.84640	1.39293
H	-0.08389	4.24779	1.16680
H	0.43998	3.29850	2.57746
C	0.61206	2.40617	-0.76422
F	-0.62120	-1.25839	-1.45928
F	0.39102	-3.17555	-1.27137
F	-1.76721	-3.04414	-1.01862
F	0.62120	1.25839	-1.45928
F	-0.39102	3.17555	-1.27137
F	1.76721	3.04414	-1.01862

Dimer CF₃/CH₃ (R/S), C-2:

-1095.26660228 Hartrees (B3LYP/6-311++G**)

C	-2.04081	0.08432	-0.04410
N	-1.37728	-0.42503	1.16752
O	-1.37546	-0.39763	-1.17290
C	-3.47413	-0.50000	-0.15789
C	-2.10519	1.61394	0.00958
H	-1.81460	-0.06325	2.01122
H	-1.44427	-1.44007	1.19319
H	-0.44962	-0.05743	-1.18175
H	-1.09126	2.00750	0.09488
H	-2.56067	1.99527	-0.90419
H	-2.68549	1.96433	0.86579
C	2.04081	-0.08432	0.04410
N	1.37728	0.42503	-1.16752
O	1.37546	0.39763	1.17290
C	3.47413	0.50000	0.15789
C	2.10519	-1.61394	-0.00958
H	1.81460	0.06325	-2.01122
H	1.44427	1.44007	-1.19319
H	0.44962	0.05743	1.18175
H	1.09126	-2.00750	-0.09488
H	2.56067	-1.99527	0.90419
H	2.68549	-1.96433	-0.86579
F	-3.46170	-1.84838	-0.17183
F	-4.11720	-0.08304	-1.25899
F	-4.22231	-0.12542	0.91293
F	3.46170	1.84838	0.17183
F	4.22231	0.12542	-0.91293
F	4.11720	0.08304	1.25899

Dimer CF₃/CH₃ (R/S), B-3:

-1095.26494124 Hartrees (B3LYP/6-311++G**)

C	0.44217	2.43472	0.25017
N	-0.88070	1.86674	0.57232
H	-1.62660	2.40621	0.13959
H	-1.01288	1.92804	1.57937
O	1.44291	1.57982	0.71081
H	1.21883	0.64128	0.51060
C	-0.36055	-1.80161	0.19992
N	0.94822	-1.26866	0.60081
H	1.70674	-1.76725	0.14438
H	1.06972	-1.36677	1.60652
O	-1.37387	-0.98367	0.71283
H	-1.17788	-0.04740	0.49039
C	-0.60623	-3.18303	0.86503
C	-0.42871	-1.94036	-1.32326
H	-0.28374	-0.95849	-1.77265
H	0.33673	-2.62044	-1.70363
H	-1.40973	-2.31843	-1.61042
C	0.69213	3.81241	0.86793
H	1.69696	4.16129	0.62981
H	-0.03646	4.54281	0.51153
H	0.60699	3.72106	1.95240
C	0.51590	2.53936	-1.29954
F	0.45862	1.32822	-1.89143
F	-0.52037	3.26906	-1.79168
F	1.64965	3.12986	-1.70631
F	-1.81236	-3.69322	0.57205
F	0.32425	-4.08066	0.44816
F	-0.50445	-3.11398	2.20917

Dimer CF₃/CH₃ (R/S), C-3:

-1095.26592869 Hartrees (B3LYP/6-311++G**)

C	-1.96081	0.66383	-0.51824
N	-1.66495	-0.42193	0.43691
O	-0.99512	0.67476	-1.52201
C	-3.32931	0.54026	-1.19197
H	-3.35975	-0.40903	-1.72972
H	-3.47686	1.34771	-1.90935
H	-4.13625	0.56178	-0.45686
C	-1.89535	1.99175	0.28974
H	-2.35078	-0.44640	1.18767
H	-1.72745	-1.30453	-0.06520
H	-0.09506	0.56395	-1.13197
C	1.96081	-0.66383	0.51824
N	1.66495	0.42193	-0.43691
O	0.99512	-0.67476	1.52201
C	3.32931	-0.54026	1.19197
H	3.35975	0.40903	1.72972
H	3.47686	-1.34771	1.90935
H	4.13625	-0.56178	0.45686
C	1.89535	-1.99175	-0.28974
H	2.35078	0.44640	-1.18767
H	1.72745	1.30453	0.06520
H	0.09506	-0.56395	1.13197
F	0.65792	-2.23411	-0.77126
F	2.73605	-1.95789	-1.35661
F	2.24425	-3.04976	0.46043
F	-2.24425	3.04976	-0.46043
F	-2.73605	1.95789	1.35661
F	-0.65792	2.23411	0.77126