Electronic Supplementary Information (ESI)

Interactions affecting $^{1}J_{C\text{-}F}$ SSCCs in neutral and ionic 2-, 3- and 4-fluoro-substituted piperidines: Normal and reverse fluorine Perlin-like effect

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Pages 2-13. Standard coordinates and absolute energies (in hartrees) for the *n*-fluoropiperidines (*n* = 2, 3 and 4) and the corresponding cations and anions, obtained at the ωB97X-D/6-311++G(d,p) level.

Atom coordinates and electronic energy (E, hartree) calculated at the ωB97X-D/6-311++G(d,p) level.

2-fluoropiperidine_Fax-Hax (neutral). E = -351.1486455

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000038913	-0.000004532	-0.000041547
2	6	0.000032126	0.000061418	-0.000007297
3	6	0.000095701	-0.000050105	0.000086090
4	6	-0.000019125	-0.000025516	0.000066161
5	6	-0.000033056	-0.000002801	0.000031004
6	1	-0.000010567	-0.000007329	-0.000019036
7	1	-0.000021979	0.000006606	-0.000000024
8	1	-0.000016779	0.000001270	0.000021453
9	1	0.000005398	0.000016464	0.000002534
10	1	-0.000004749	-0.000023415	-0.000009533
11	1	0.000023188	0.000000952	-0.000010720
12	1	0.000009824	0.000005404	-0.000007909
13	1	0.000028411	0.000019012	0.000016125
14	7	-0.000014858	-0.000073611	0.000016984
15	1	-0.000008960	0.000012687	-0.000036565
16	9	-0.000020753	0.000030069	-0.000078805
17	1	-0.000004909	0.000033428	-0.000028914

2-fluoropiperidine_Fax-Heq (neutral). E = -351.1566855

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000017371	-0.000003373	-0.000020294
2	6	0.000018789	-0.000021837	-0.000005674
3	6	0.000001061	-0.000012886	-0.000016556
4	6	-0.000009695	0.000004464	0.000054130
5	6	-0.000013869	-0.000018684	0.000029035
6	1	-0.000001593	0.000014157	-0.000024715
7	1	-0.000011478	0.000021206	-0.000005291
8	1	-0.000006378	0.000001394	0.000015990
9	1	0.000002704	0.000010963	-0.000002243
10	1	-0.000004877	-0.000014023	0.000004946
11	1	0.000006304	-0.000009317	0.000000804
12	1	0.000008017	0.000002158	-0.000008804
13	1	0.000016513	0.000001308	0.000013903
14	7	-0.000019973	0.000008597	-0.000017515
15	1	0.000018023	0.000002983	-0.000021291
16	1	-0.000006480	0.000010172	-0.000007814
17	9	0.000020303	0.000002718	0.000011387

2-fluoropiperidine_Feq-Hax (neutral). E = -351.147973

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000026271	-0.000004380	0.000008118
2	6	-0.000061274	-0.000060132	-0.000039225
3	6	-0.000096168	-0.000002881	-0.000012870
4	6	0.000059425	-0.000032807	-0.000000817
5	6	-0.000035420	-0.000038114	0.000004750
6	1	0.000014646	0.000035081	-0.000034497
7	1	0.000014625	0.000037853	-0.000003283
8	1	0.000003728	-0.000000038	0.000002764
9	1	-0.000003174	0.000022828	-0.000030617
10	1	0.000012721	0.000008333	-0.000032372
11	1	-0.000000775	-0.000011735	-0.000017600
12	1	0.000019185	-0.000010122	0.000015130
13	7	0.000090814	-0.000023042	0.000071540
14	1	-0.000003953	0.000011908	0.000013624
15	1	-0.000033171	0.000047301	-0.000030358
16	9	0.000016275	0.000026405	0.000031944
17	1	-0.000023755	-0.000006458	0.000053770

2-fluoropiperidine_Feq-Heq (neutral). E = -351.1492855

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000068827	0.000042614	0.000030297
2	6	-0.000064342	-0.000077280	0.000027935
3	6	-0.000077080	-0.000052207	0.000028397
4	6	0.000069210	-0.000073006	-0.000012825
5	6	-0.000035316	-0.000027596	-0.000015984
6	1	0.000024725	0.000028214	-0.000049896
7	1	0.000013433	0.000057499	-0.000016730
8	1	-0.000019900	-0.000004775	0.000000241
9	1	0.000013387	0.000007714	-0.000035915
10	1	0.000009341	0.000013210	-0.000039922
11	1	0.000006783	-0.000024445	-0.000002893
12	1	0.000016988	-0.000030185	0.000023412
13	7	-0.000041670	0.000078937	-0.000015938
14	1	0.000034277	-0.000002995	0.000003062
15	1	-0.000022406	0.000013637	0.000022380
16	1	-0.000017745	-0.000004339	0.000045853
17	9	0.000021488	0.000055003	0.000008526

2-fluoropiperidine_Fax (cation). E = -351.5156028

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000009583	0.000005449	-0.000007207
2	6	-0.000001549	0.000012894	0.000016427
3	6	-0.000009218	-0.000023789	-0.000041079
4	6	-0.000031916	0.000008030	-0.000022136
5	6	-0.000007496	-0.000009033	-0.000002935
6	1	0.000009207	0.000004399	0.000013296
7	1	0.000028492	-0.000004131	0.000013934
8	1	0.000016880	-0.000010929	-0.000006491
9	1	0.000012858	-0.000005390	-0.000006067
10	1	-0.000011792	0.000000558	-0.000015983
11	1	-0.000008301	-0.000007222	-0.000015788
12	1	-0.000018039	0.000008772	-0.000014455
13	1	-0.000007908	-0.000004292	-0.000024551
14	7	0.000001622	0.000016124	0.000052183
15	9	0.000000017	-0.000000052	0.000030097
16	1	-0.000005432	0.000011463	0.000003560
17	1	0.000004221	0.000005514	0.000018772
18	1	0.000018771	-0.000008365	0.000008426

2-fluoropiperidine_Feq (cation). E = -351.5163837

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000017359	-0.000019531	0.000015475
2	6	0.000034059	0.000108456	0.000011055
3	6	-0.000072287	-0.000016737	0.000070261
4	6	0.000069614	0.000068363	0.000013218
5	6	0.000014534	-0.000043150	-0.000043861
6	1	0.000002442	-0.000028467	-0.000019048
7	1	-0.000007920	-0.000001304	-0.000023070
8	1	0.000002171	0.000005915	-0.000011034
9	1	-0.000002664	0.000007826	-0.000001643
10	1	-0.000005254	-0.000039558	0.000021407
11	1	-0.000005252	-0.000000900	0.000014686
12	1	0.000006390	-0.000011092	0.000009403
13	1	0.000007983	0.000003769	0.000006958
14	7	0.000029232	0.000002423	-0.000111883
15	1	-0.000033938	-0.000009191	0.000032733
16	1	-0.000018633	-0.000017351	0.000038580
17	1	0.000002093	0.000001068	-0.000008129
18	9	-0.000005212	-0.000010539	-0.000015108

2-fluoropiperidine_Fax (anion). Not converged.

2-fluoropiperidine_Feq (anion). E = -350.5215934

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000133083	-0.000068424	-0.000056736
2	6	-0.000068246	0.000026130	0.000018561
3	6	-0.000000732	-0.000122836	-0.000061635
4	6	0.000113945	0.000036209	-0.000022372
5	6	-0.000125408	-0.000050048	0.000075683
6	1	-0.000002917	0.000026385	-0.000035087
7	1	-0.000000289	0.000056804	0.000024033
8	1	0.000001789	-0.000003454	0.000012867
9	1	-0.000037166	0.000039695	-0.000036299
10	1	-0.000006408	-0.000005802	0.000003430
11	1	-0.000030616	-0.000013078	-0.000016636
12	1	-0.000022151	0.000016204	0.000044936
13	1	0.000008914	-0.000004597	-0.000022291
14	1	0.000073562	0.000002295	0.000010177
15	9	-0.000037463	-0.000025833	-0.000004267
16	7	0.000000101	0.000090349	0.000065636

3-fluoropiperidine_Fax-Hax (neutral). E = -351.1451717

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000019986	-0.000003456	0.000002197
2	6	-0.000077881	-0.000060876	-0.000014814
3	6	-0.000114214	0.000083789	0.000080561
4	6	0.000045858	-0.000054362	0.000061318
5	6	-0.000005435	-0.000002478	0.000038028
6	1	0.000025692	0.000055595	-0.000040794
7	1	0.000003979	0.000036524	0.000002468
8	1	-0.000002571	-0.000030740	0.000024890
9	1	0.000007183	0.000006649	0.000001636
10	1	0.000019194	-0.000001186	-0.000077533
11	1	-0.000007258	-0.000021457	-0.000022962
12	1	-0.000009462	-0.000014471	-0.000006640
13	1	0.000004565	-0.000006397	-0.000010044
14	1	0.000028360	-0.000017508	0.000030179
15	7	0.000158369	-0.000032762	0.000026407
16	1	-0.000064071	0.000041242	-0.000055464
17	9	-0.000032296	0.000021894	-0.000039434

3-fluoropiperidine_Fax-Heq (neutral). E = -351.1424806

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000028012	0.000038652	-0.000009502
2	6	-0.000034855	0.000011476	0.000011576
3	6	-0.000031126	0.000004403	0.000051264
4	6	0.000033306	-0.000055241	0.000025835
5	6	0.000011753	0.000019839	0.000014501
6	1	0.000004676	-0.000001672	-0.000017894
7	1	0.000003117	0.000006479	-0.000012581
8	1	-0.000014654	-0.000025834	0.000012224
9	1	0.000010596	-0.000012097	0.000006743
10	1	0.000015169	0.000006795	-0.000019742
11	1	-0.000007062	-0.000005453	-0.000000060
12	1	0.000000483	-0.000009192	0.000004299
13	1	-0.000011198	-0.000016767	-0.000000691
14	1	0.000008904	0.000000906	0.000012032
15	7	-0.000019273	0.000007046	-0.000051818
16	9	-0.000023833	0.000030234	-0.000035303
17	1	0.000025986	0.000000426	0.000009116

3-fluoropiperidine_Feq-Hax (neutral). E = -351.1438128

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000010795	-0.000011993	0.000009788
2	6	-0.000047018	-0.000043061	-0.000006788
3	6	-0.000074689	0.000041276	0.000043326
4	6	0.000051778	-0.000063231	-0.000046675
5	6	0.000014908	-0.000002813	-0.000028795
6	1	0.000013370	0.000037798	0.000004570
7	1	0.000023768	0.000015844	0.000026339
8	1	0.000023362	-0.000018449	0.000002617
9	1	0.000000393	-0.000000299	-0.000002959
10	1	-0.000015552	0.000009909	-0.000021547
11	1	-0.000005895	-0.000010160	-0.000013727
12	1	-0.000020164	0.000016157	-0.000009531
13	1	0.000001242	-0.000008034	-0.000011923
14	7	0.000110089	-0.000026421	0.000047763
15	1	-0.000012830	0.000006537	-0.000011719
16	9	-0.000053283	0.000039706	0.000050095
17	1	-0.000020274	0.000017233	-0.000030836

3-fluoropiperidine_Feq-Heq (neutral). E = -351.1446525

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000022090	0.000011112	0.000023308
2	6	-0.000037038	-0.000026205	0.000022720
3	6	-0.000047626	0.000005673	0.000031844
4	6	0.000048942	-0.000032876	-0.000022381
5	6	0.000017981	-0.000005183	-0.000051614
6	1	0.000001433	0.000006709	0.000002918
7	1	0.000011199	-0.000008320	0.000020410
8	1	0.000004040	-0.000036588	0.000013441
9	1	0.000002737	-0.000012117	0.000014286
10	1	-0.000007428	0.000027864	-0.000013535
11	1	0.000003906	-0.000005054	-0.000030879
12	1	-0.000016009	0.000021375	0.000010950
13	1	0.000008350	-0.000000101	0.000005653
14	7	-0.000021433	0.000017883	-0.000053175
15	1	0.000047014	-0.000007206	0.000026264
16	1	-0.000023259	0.000007431	-0.000021794
17	9	-0.000014898	0.000035602	0.000021586

3-fluoropiperidine_Fax (cation). E = -351.5194527

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000008549	-0.000044289	-0.000026406
2	6	0.000014178	0.000067678	0.000013155
3	6	-0.000099539	-0.000015861	-0.000050759
4	6	0.000056206	-0.000037431	0.000067844
5	6	0.000001444	0.000033289	-0.000003641
6	1	0.000001781	-0.000023508	-0.000017210
7	1	-0.000008747	-0.000008727	0.000003288
8	1	0.000012408	0.000000804	0.000012130
9	1	0.000012762	-0.000006371	-0.000000758
10	1	-0.000005036	0.000015718	-0.000009167
11	1	0.000008414	0.000001412	-0.000004872
12	1	0.000009425	0.000004808	0.000028495
13	1	0.000004799	0.000005090	-0.000002916
14	1	0.000004327	-0.000021018	0.000008278
15	7	-0.000047570	0.000033173	-0.000030358
16	1	0.000010649	0.000006189	0.000023573
17	1	0.000013814	0.000009769	0.000011459
18	9	0.000019234	-0.000020725	-0.000022136

3-fluoropiperidine_Feq (cation). E = -351.5112594

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000003387	-0.000011685	0.000001377
2	6	0.000006969	0.000035092	0.000015814
3	6	-0.000028435	0.000001315	-0.000027277
4	6	0.000003041	0.000007323	0.000010843
5	6	0.000001265	-0.000011036	-0.000015658
6	1	0.000002741	-0.000001960	0.000009367
7	1	0.000008529	-0.000017985	0.000021282
8	1	0.000009329	-0.000015935	0.000008477
9	1	0.000011682	-0.000007774	0.000012412
10	1	-0.000000675	0.000021894	-0.000000118
11	1	0.000003009	0.000004582	-0.000010288
12	1	-0.000006075	0.000012678	0.000003435
13	1	0.000001047	-0.000001972	-0.000001052
14	7	-0.000010030	-0.000025030	-0.000000855
15	1	0.000005730	-0.000004475	0.000003618
16	1	0.000003060	0.000007180	0.000011476
17	9	0.000003698	0.000007931	-0.000020271
18	1	-0.000011498	-0.000000144	-0.000022581

3-fluoropiperidine_Fax (anion). E = -350.5053566

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000084412	-0.000010027	-0.000038500
2	6	0.000007811	0.000010672	0.000053347
3	6	-0.000003115	-0.000045611	0.000067015
4	6	0.000088666	-0.000005802	0.000083537
5	6	-0.000067095	-0.000030052	0.000016059
6	1	-0.000004138	0.000022465	-0.000009895
7	1	0.000023927	0.000034220	0.000006501
8	1	-0.000010641	-0.000019184	0.000010199
9	1	0.000019433	-0.000001551	0.000002383
10	1	-0.000032840	0.000030366	-0.000037492
11	1	-0.000016563	-0.000009516	-0.000018095
12	1	-0.000025515	-0.000014132	-0.000016808
13	1	0.000023845	0.000003703	-0.000006449
14	1	0.000019594	-0.000021733	0.000004987
15	7	-0.000031299	0.000014600	-0.000039817
16	9	-0.000076482	0.000041581	-0.000076972

3-fluoropiperidine_Feq (anion). E = -350.5115927

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000143082	-0.000047841	-0.000021824
2	6	-0.000082061	-0.000104200	0.000029530
3	6	-0.000002723	0.000013287	0.000067256
4	6	0.000152666	-0.000035051	0.000040818
5	6	-0.000112232	-0.000047595	0.000021916
6	1	-0.000031534	0.000040917	-0.000034815
7	1	0.000016598	0.000022442	0.000034164
8	1	0.000021563	-0.000019095	0.000030074
9	1	-0.000044221	0.000021717	-0.000012130
10	1	-0.000036548	0.000014762	-0.000040430
11	1	0.000000436	-0.000034055	-0.000028727
12	1	-0.000010756	0.000025987	-0.000026415
13	1	0.000031243	0.000012235	0.000006775
14	7	0.000048408	0.000037769	-0.000026383
15	9	-0.000068839	0.000058618	0.000068504
16	1	-0.000025081	0.000040103	-0.000108314

4-fluoropiperidine_Fax-Hax (neutral). E = -351.1441981

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000102801	0.000026895	-0.000015378
2	6	0.000001357	0.000006187	0.000013181
3	6	-0.000020452	0.000029220	-0.000053698
4	6	0.000015012	0.000000111	0.000006605
5	6	-0.000034766	0.000081529	0.000063015
6	1	-0.000007271	0.000019569	-0.000011846
7	1	-0.000039057	0.000013261	-0.000021358
8	1	-0.000019925	-0.000000415	0.000012808
9	1	-0.000004041	-0.000012910	0.000002511
10	1	0.000003846	0.000015786	-0.000018124
11	1	-0.000009742	-0.000016239	0.000013712
12	1	0.000004608	-0.000004190	-0.000046424
13	1	0.000016946	-0.000014385	-0.000008324
14	1	0.000005003	-0.000022343	0.000005727
15	7	-0.000026548	-0.000140333	0.000048502
16	1	-0.000008043	0.000036847	-0.000039247
17	9	0.000020271	-0.000018592	0.000048339

4-fluoropiperidine_Fax-Heq (neutral). E = -351.1454491

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000025460	-0.000011527	0.000012938
2	6	-0.000002805	-0.000015370	0.000004751
3	6	-0.000017948	0.000009371	-0.000038072
4	6	-0.000003239	-0.000015536	0.000004998
5	6	-0.000005522	0.000000729	0.000030468
6	1	0.000000149	-0.000000120	-0.000007547
7	1	-0.000003918	0.000004831	-0.000001452
8	1	-0.000004678	0.000004200	0.000002880
9	1	-0.000006019	0.000002353	-0.000004077
10	1	0.000004904	0.000003246	0.000000513
11	1	0.000002928	0.000002315	-0.000005334
12	1	0.000006055	0.000000019	-0.000003242
13	1	0.000000121	0.000004989	0.000003017
14	7	-0.000006397	0.000028566	-0.000031638
15	1	-0.000003244	-0.000016963	0.000005940
16	9	0.000009915	-0.000007165	0.000022618
17	1	0.000004237	0.000006062	0.000003238

4-fluoropiperidine_Feq-Hax (neutral). E = -351.1450951

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000089303	0.000036831	-0.000024590
2	6	-0.000014195	-0.000018389	0.000025094
3	6	-0.000042805	-0.000063872	-0.000029488
4	6	0.000016228	-0.000030765	0.000008546
5	6	-0.000031856	0.000084116	0.000044431
6	1	-0.000009890	0.000005699	0.000001151
7	1	-0.000046990	0.000002485	-0.000027609
8	1	-0.000014195	0.000006635	-0.000004647
9	1	0.000007598	-0.000000700	-0.000008582
10	1	0.000008293	0.000004686	0.000027479
11	1	-0.000002970	-0.000014694	-0.000052979
12	1	0.000005096	-0.000000497	-0.000015908
13	1	0.000020158	-0.000000054	0.000020949
14	7	-0.000016949	-0.000126190	0.000056411
15	1	-0.000012913	0.000054111	-0.000060262
16	1	0.000008026	-0.000015912	0.000024673
17	9	0.000038061	0.000076509	0.000015332

4-fluoropiperidine_Feq-Heq (neutral). E = -351.1452919

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000036803	0.000124757	0.000109664
2	6	-0.000162339	0.000049597	0.000110196
3	6	-0.000108160	-0.000385151	0.000080886
4	6	0.000175345	-0.000080651	-0.000075024
5	6	0.000136104	0.000085441	0.000054295
6	1	0.000023716	-0.000035916	0.000017028
7	1	-0.000001264	-0.000045949	-0.000006181
8	1	-0.000049519	-0.000021425	-0.000054546
9	1	-0.000014538	-0.000020169	0.000038308
10	1	-0.000024125	0.000051234	0.000000677
11	1	-0.000029612	-0.000034954	0.000009588
12	1	-0.000035549	-0.000025840	-0.000062314
13	1	0.000036863	0.000028958	-0.000032360
14	7	-0.000071566	-0.000062820	-0.000086110
15	1	-0.000041117	0.000056282	-0.000112993
16	9	0.000095739	0.000248610	-0.000000954
17	1	0.000033219	0.000067997	0.000009840

4-fluoropiperidine_Fax (cation). E = -351.5193963

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000018552	0.000006380	0.000006918
2	6	0.000009195	0.000040059	0.000002760
3	6	0.000017318	-0.000026639	-0.000025379
4	6	-0.000035887	-0.000014510	-0.000004384
5	6	0.000003766	0.000007010	-0.000009167
6	1	0.000012970	0.000001037	-0.000020210
7	1	-0.000007774	-0.000004776	0.000004520
8	1	-0.000005390	-0.000006354	0.000006991
9	1	0.000018062	0.000001033	-0.000003213
10	1	0.000019086	0.000002757	-0.000002408
11	1	-0.000004878	-0.000001386	0.000009032
12	1	0.000007660	-0.000006385	0.000012067
13	7	-0.000017119	-0.000008074	-0.000004428
14	1	-0.000004293	0.000021659	-0.000003080
15	1	-0.000003316	-0.000000892	0.000001555
16	1	-0.000010859	-0.000000285	0.000001493
17	9	0.000005093	-0.000011310	0.000023302
18	1	0.000014917	0.000000677	0.000003629

4-fluoropiperidine_Feq (cation). E = -351.5143783

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002594	0.000014683	0.000006213
2	6	0.000003123	0.000027621	-0.000002801
3	6	0.000012400	-0.000014030	-0.000016981
4	6	-0.000014283	-0.000017593	-0.000008349
5	6	0.000001917	0.000001825	0.000001704
6	1	0.000010072	-0.000000644	-0.000010966
7	1	-0.000004848	-0.000004839	-0.000004284
8	1	-0.000009148	-0.000006322	0.000005397
9	1	0.000013409	-0.000004087	0.000004731
10	1	0.000014223	-0.000001816	0.000005729
11	1	-0.000008394	-0.000000750	0.000007096
12	7	-0.000026888	-0.000010657	0.000006836
13	1	-0.000003619	0.000018418	-0.000003797
14	1	-0.000003376	0.000005926	-0.000010936
15	1	-0.000004092	0.000002523	-0.000003563
16	1	0.000009636	0.000002885	-0.000000811
17	9	0.000001555	-0.000005281	0.000009907
18	1	0.000010907	-0.000007862	0.000014876

4-fluoropiperidine_Fax (anion). E = -350.5045158

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000075281	-0.000040787	-0.000030173
2	6	-0.000047620	-0.000041668	-0.000007242
3	6	-0.000091347	0.000005469	0.000024756
4	6	0.000079103	0.000047153	0.000014194
5	6	-0.000043504	0.000039664	-0.000078282
6	1	-0.000011976	0.000018934	-0.000031720
7	1	0.000000640	0.000007837	0.000002689
8	1	-0.000004022	-0.000002086	0.000027720
9	1	-0.000028633	0.000002465	-0.000002746
10	1	-0.000029121	-0.000000007	-0.000004805
11	1	0.000001404	-0.000020473	0.000016886
12	1	0.000019179	-0.000014965	0.000026091
13	7	0.000048637	0.000000728	-0.000023155
14	1	0.000019368	0.000044851	-0.000010825
15	9	0.000010362	-0.000042782	0.000084961
16	1	0.000002249	-0.000004333	-0.000008349

4-fluoropiperidine_Feq (anion). E = -350.5126689

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000061440	0.000025025	-0.000010274
2	6	-0.000118288	-0.000275863	0.000083449
3	6	-0.000169837	-0.000025885	0.000330041
4	6	0.000041536	-0.000015072	-0.000020408
5	6	0.000435503	-0.000010875	0.000034379
6	1	-0.000033252	0.000154829	-0.000145084
7	1	-0.000027295	0.000119535	0.000017571
8	1	0.000039834	-0.000070610	0.000088394
9	1	-0.000026134	0.000028254	-0.000004091
10	1	-0.000040885	0.000022063	-0.000200706
11	1	-0.000031250	-0.000009010	-0.000023501
12	1	0.000040517	-0.000031877	0.000106911
13	1	-0.000015745	0.000027163	-0.000050532
14	7	0.000243599	0.000018647	-0.000135395
15	9	-0.000417940	-0.000012387	0.000033609
16	1	0.000018194	0.000056062	-0.000104363