An extensive investigation of Reactions Involved in the Nitrogen Trifluoride Dissociation

Simone S. Ramalho[‡], Wiliam F. da Cunha[†], Alessandra F. Albernaz[†], Pedro H. O. Neto[†], Geraldo Magela e Silva[†], and Ricardo Gargano[†]
‡ *Goias Federal Institute of Education, Science and Technology, Brazil and*
† *Institute of Physics, University of Brasilia, Brasilia, 70.919-970, Brazil*
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[1] P. R. P. Barreto, A. F. A. Vilela, R. Gargano, *Int. J. Quantum Chem.*, 2005, **103** 659.

TABLE I: Total electronic energies(hartree), forward barrier($V_f + d\varepsilon_{ZPE}$), reverse barrier($V_r + d\varepsilon_{ZPE}$), and enthalpy with ZPE correction($\Delta H + d\varepsilon_{ZPE}$) and experimental heat of reaction ($\Delta_f H^0$(exp) values, given in kcal mol^{-1}, using Dunning basis set for reactant, product and TS for NF_3+F=NF_2+F_2 reaction.

	$NF_3 + F$	TS	$NF_2 + F_2$	$V_f + d\varepsilon_{ZPE}$	$V_r + d\varepsilon_{ZPE}$	$\Delta H + d\varepsilon_{ZPE}$
MP2/cc-pVDZ	-452.8164999	-452.7238979	-452.7786090	55.8130	33.2888	22.5242
MP2/aug-cc-pVDZ	-452.9343944	-452.8313556	-452.8916510	62.3622	36.7930	25.5692
MP2/cc-pVTZ	-453.3114885	-453.2069447	-453.2725274	63.3066	40.1109	23.1958
MP2/aug-cc-pVTZ	-453.3570794	-453.2510599	-453.3172341	64.2326	40.4820	23.7506
MP4(SDTQ)/cc-pVDZ	-452.8615325	-452.7805737	-452.8256230	48.5068	27.2260	21.2809
MP4(SDTQ)/aug-cc-pVDZ	-452.9894745	-452.9006373	-452.9487486	53.4506	29.1474	24.3032
MP4(SDTQ)/cc-pVTZ	-453.3717335	-453.2792837	-453.3348592	55.7175	33.8312	21.8863
MP4(SDTQ)/aug-cc-pVTZ	-453.4218449		-453.3841565			22.3971
QCISD(T)/cc-pVDZ	-452.8589287	-452.8195527	-452.8258868	22.4132	2.9318	19.4814
QCISD(T)/aug-cc-pVDZ	-452.9849417		-452.9457505			23.3402
QCISD(T)/cc-pVTZ	-453.3649491		-453.3297451			20.8381
QCISD(T)/aug-cc-pVTZ	-453.4141924		-453.3776506			21.6776
CCSD(T)/cc-pVDZ	-452.8575819	-452.8175282	-452.8245663	22.8385	3.3736	19.4649
CCSD(T)/aug-cc-pVDZ	-452.9830006		-452.9438843			23.2931
CCSD(T)/cc-pVTZ	-453.3630415		-453.3277174			20.9135
CCSD(T)/aug-cc-pVTZ	-453.4120261		-453.3753723			21.7479
$d\varepsilon_{ZPE}$	6.3256	4.0300	5.0729			-1.2527

TABLE II: Total electronic energies(hartree), forward barrier($V_f + d\varepsilon_{ZPE}$), reverse barrier($V_r + d\varepsilon_{ZPE}$), and enthalpy with ZPE correction($\Delta H + d\varepsilon_{ZPE}$) and experimental heat of reaction ($\Delta_f H^0$(exp) values, given in kcal mol^{-1}, using Pople basis set for reactant, product and TS for NF_3+F=NF_2+F_2 reaction.

	$NF_3 + F$	TS	$NF_2 + F_2$	$V_f + d\varepsilon_{ZPE}$	$V_r + d\varepsilon_{ZPE}$	$\Delta H + d\varepsilon_{ZPE}$
MP2/6-31G(d)	-452.7158157	-452.6283527	-452.6816125	52.9515	32.6692	20.2823
MP2/6-31++G(d.p)	-452.7719942	-452.6716458	-452.7323849	61.0372	37.3626	23.6746
MP2/6-311++G(d.p)	-453.1010575	-453.0022258	-453.0582130	60.0855	34.3807	25.7048
MP2/6-311++G(df.pd)	-453.2204930	-453.1149061	-453.1748885	64.3244	36.8877	27.4367
MP2/6-311++G(3df.3pd)	-453.3576485	-453.2499220	-453.3150530	65.6670	40.1185	25.5485
MP4(SDTQ)/6-31G(d)	-452.7707988	-452.6845549	-452.7347373	52.1865	30.7381	21.4484
MP4(SDTQ)/6-31++G(d.p)	-452.8204531	-452.7316474	-452.7810884	53.7941	30.2729	23.5212
MP4(SDTQ)/6-311++G(d.p)	-453.1532972		-453.1128127			24.2238
MP4(SDTQ)/6-311++G(df.pd)	-453.2805706		-453.2374394			25.8847
MP4(SDTQ)/6-311++G(3df.3pd)	-453.4242297		-453.3836737			24.2687
QCISD(T)/6-31G(d)	-452.7670276		-452.7336563			19.7602
QCISD(T)/6-31++G(d.p)	-452.8152703		-452.7776288			22.4398
QCISD(T)/6-311++G(d.p)	-453.1488963		-453.1099966			23.2294
QCISD(T)/6-311++G(df.pd)	-453.2752299		-453.2340658			24.6503
CCSD(T)/6-31G(d)	-452.7653505		-452.7321047			19.6815
CCSD(T)/6-31++G(d.p)	-452.8131630		-452.7756542			22.3566
CCSD(T)/6-311++G(d.p)	-453.1468068		-453.1077868			23.3049
CCSD(T)/6-311++G(df.pd)	-453.2732259		-453.2319374			24.7284
$d\varepsilon_{ZPE}$	6.3513	4.4190	5.1708			-1.1806
$\Delta_f H^0$(exp)[1]	-11.733		8.300			20.033

TABLE III: Total electronic energies(hartree), forward barrier($V_f + d\varepsilon_{ZPE}$), reverse barrier($V_r + d\varepsilon_{ZPE}$), and enthalpy with ZPE correction($\Delta H + d\varepsilon_{ZPE}$) and experimental heat of reaction ($\Delta_f H^0$(exp) values, given in kcal mol^{-1}, using Dunning and Pople basis set for reactant, product and TS for NF_3+F=NF_3+F reaction.

	$NF_3 + F$	TS	$NF_3 + F$	$V_f + d\varepsilon_{ZPE}$	$V_r + d\varepsilon_{ZPE}$	$\Delta H + d\varepsilon_{ZPE}$
MP2/cc-pVDZ	-452.8164999	-452.7654434	-452.8164999	32.6894	32.6894	0.0000
MP2/aug-cc-pVDZ	-452.9343944	-452.8935552	-452.9343944	26.2780	26.2780	0.0000
MP2/cc-pVTZ	-453.3114885	-453.2720529	-453.3114885	25.3972	25.3972	0.0000
MP2/aug-cc-pVTZ	-453.3570794	-453.3230592	-453.3570794	21.9990	21.9990	0.0000
MP4(SDTQ)/cc-pVDZ	-452.8615325	-452.8129134	-452.8615325	31.1599	31.1599	0.0000
MP4(SDTQ)/aug-cc-pVDZ	-452.9894745	-452.9531076	-452.9894745	23.4716	23.4716	0.0000
MP4(SDTQ)/cc-pVTZ	-453.3717335	-453.2713335	-453.3717335	63.6530	63.6529	0.0000
MP4(SDTQ)/aug-cc-pVTZ	-453.4218449		-453.4218449			0.0000
QCISD(T)/cc-pVDZ	-452.8589287	-452.8199164	-452.8589287	25.1316	25.1316	0.0000
QCISD(T)/aug-cc-pVDZ	-452.9849417	-452.9575320	-452.9849417	17.8508	17.8508	0.0000
QCISD(T)/cc-pVTZ	-453.3649491		-453.3649491			0.0000
QCISD(T)/aug-cc-pVTZ	-453.4141924		-453.4141924			0.0000
CCSD(T)/cc-pVDZ	-452.8575819	-452.8176296	-452.8575819	25.7214	25.7214	0.0000
CCSD(T)/aug-cc-pVDZ	-452.9830006		-452.9830006			0.0000
CCSD(T)/cc-pVTZ	-453.3630415		-453.3630415			0.0000
CCSD(T)/aug-cc-pVTZ	-453.4120261		-453.4120261			0.0000
$d\varepsilon_{ZPE}$	6.3256	6.9766	6.3256			0.0000
MP2/6-31G(d)	-452.7158157	-452.6841477	-452.7158157	20.8651	20.8651	0.0000
MP2/6-31++G(d.p)	-452.7719942	-452.7298857	-452.7719942	27.4166	27.4166	0.0000
MP2/6-311++G(d.p)	-453.1010575	-453.0529974	-453.1010575	31.1513	31.1513	0.0000
MP2/6-311++G(df.pd)	-453.2204930	-453.1769466	-453.2204930	28.3189	28.3189	0.0000
MP2/6-311++G(3df.3pd)	-453.3576485	-453.3213460	-453.3576485	23.7733	23.7733	0.0000
MP4(SDTQ)/6-31G(d)	-452.7707988	-452.7310447	-452.7707988	25.9392	25.9392	0.0000
MP4(SDTQ)/6-31++G(d.p)	-452.8204531	-452.7808896	-452.8204531	25.8196	25.8196	0.0000
MP4(SDTQ)/6-311++G(d.p)	-453.1532972	-453.1088523	-453.1532972	28.8827	28.8827	0.0000
MP4(SDTQ)/6-311++G(df.pd)	-453.2805706	-453.2408221	-453.2805706	25.9357	25.9357	0.0000
MP4(SDTQ)/6-311++G(3df.3pd)	-453.4242297		-453.4242297			0.0000
QCISD(T)/6-31G(d)	-452.7670276	-452.7356302	-452.7670276	20.6953	20.6953	0.0000
QCISD(T)/6-31++G(d.p)	-452.8152703	-452.7841483	-452.8152703	20.5225	20.5225	0.0000
QCISD(T)/6-311++G(d.p)	-453.1488963	-453.1137090	-453.1488963	23.0735	23.0735	0.0000
QCISD(T)/6-311++G(df.pd)	-453.2752299		-453.2752299			0.0000
CCSD(T)/6-31G(d)	-452.7653505	-452.7330607	-452.7653505	21.2553	21.2553	0.0000
CCSD(T)/6-31++G(d.p)	-452.8131630	-452.7810081	-452.8131630	21.1707	21.1706	0.0000
CCSD(T)/6-311++G(d.p)	-453.1468068	-453.1104789	-453.1468068	23.7892	23.7892	0.0000
CCSD(T)/6-311++G(df.pd)	-453.2732259		-453.2732259			0.0000
$d\varepsilon_{ZPE}$	6.3513	7.3445	6.3513			0.0000
$\Delta_f H^0$(exp)[1]	-11.733		-11.733			0.000

TABLE IV: Total electronic energies(hartree), forward barrier($V_f + d\varepsilon_{ZPE}$), reverse barrier($V_r + d\varepsilon_{ZPE}$), and enthalpy with ZPE correction($\Delta H + d\varepsilon_{ZPE}$) and experimental heat of reaction ($\Delta_f H^0$(exp) values, given in kcal mol^{-1}, using Dunning and Pople basis set for reactant, product and TS for $N_2F = N_2$+F reaction.

	N_2F	TS_{10}	$N_2 + F$	$V_d + d\varepsilon_{ZPE}$	$V_r + d\varepsilon_{ZPE}$	$\Delta H + d\varepsilon_{ZPE}$
MP2/cc-pVDZ	-208.5517426	-208.5337965	-208.7849231	10.5746	158.2398	-147.6652
MP2/aug-cc-pVDZ	-208.6027351	-208.5835283	-208.8230135	11.3657	150.9347	-139.5690
MP2/cc-pVTZ	-208.7792194	-208.7595070	-208.9998415	11.6830	151.4676	-139.7847
MP2/aug-cc-pVTZ	-208.8020345	-208.7827424	-209.0182104	11.4192	148.4139	-136.9947
MP4(SDTQ)/cc-pVDZ	-208.5949819	-208.5772704	-208.8135452	10.4274	148.9201	-138.4928
MP4(SDTQ)/aug-cc-pVDZ	-208.6508216	-208.6318322	-208.8555815	11.2293	141.0603	-129.8310
MP4(SDTQ)/cc-pVTZ	-208.8301623	-208.8106211	-209.0372541	11.5755	142.8698	-131.2943
MP4(SDTQ)/aug-cc-pVTZ	-208.8550659	-208.8357632	-209.0565876	11.4259	139.2249	-127.7990
QCISD(T)/cc-pVDZ	-208.5915661	-208.5843397	-208.8098404	3.8479	142.1593	-138.3114
QCISD(T)/aug-cc-pVDZ	-208.6458403	-208.6375966	-208.8518604	4.4863	135.1080	-130.6218
QCISD(T)/cc-pVTZ	-208.8236503	-208.8153371	-209.0307763	4.5299	135.8456	-131.3158
QCISD(T)/aug-cc-pVTZ			-209.0500510			
CCSD(T)/cc-pVDZ	-208.5900516	-208.5829576	-208.8093426	3.7648	142.7142	-138.9494
CCSD(T)/aug-cc-pVDZ	-208.6441067	-208.6359908	-208.8513096	4.4061	135.7701	-131.3640
CCSD(T)/cc-pVTZ	-208.8217596	-208.8135499	-209.0300555	4.4649	136.5148	-132.0499
CCSD(T)/aug-cc-pVTZ			-209.0493049			
$d\varepsilon_{ZPE}$	4.3845	3.6978	3.0423			-1.3422
MP2/6-31G(d)	-208.5229701	-208.5091477	-208.7506130	7.9671	152.1963	-144.2292
MP2/6-31++G(d.p)	-208.5464668	-208.5273840	-208.7696058	11.2681	152.6710	-141.4030
MP2/6-311++G(d.p)	-208.6808513	-208.6663592	-208.9169090	8.3874	157.8969	-149.5096
MP2/6-311++G(df.pd)	-208.7410055	-208.7244270	-208.9683369	9.6966	153.7303	-144.0338
MP2/6-311++G(3df.3pd)	-208.8065405	-208.7885230	-209.0254932	10.5996	149.3756	-138.7761
MP4(SDTQ)/6-31G(d)	-208.5741141	-208.5523847	-208.7791967	12.9288	143.0012	-130.0724
MP4(SDTQ)/6-31++G(d.p)	-208.5913021	-208.5720557	-208.7990214	11.3707	143.0977	-131.7270
MP4(SDTQ)/6-311++G(d.p)	-208.7287835	-208.7138889	-208.9492587	8.6399	148.3713	-139.7314
MP4(SDTQ)/6-311++G(df.pd)	-208.7925163	-208.7756336	-209.0039361	9.8875	143.9365	-134.0491
MP4(SDTQ)/6-311++G(3df.3pd)	-208.8608898	-208.8425388	-209.0653474	10.8089	140.4891	-129.6802
QCISD(T)/6-31G(d)	-208.5693075	-208.5590679	-208.7752195	5.7189	136.3117	-130.5929
QCISD(T)/6-31++G(d.p)	-208.5855687	-208.5780340	-208.7947996	4.0215	136.6970	-132.6755
QCISD(T)/6-311++G(d.p)	-208.7237157	-208.7206054	-208.9436550	1.2452	140.6403	-139.3952
QCISD(T)/6-311++G(df.pd)	-208.7869143	-208.7818969	-208.9978573	2.4419	136.1918	-133.7499
CCSD(T)/6-31G(d)	-208.5677199	-208.5575821	-208.7746424	5.6550	136.8820	-131.2270
CCSD(T)/6-31++G(d.p)	-208.5838115	-208.5763930	-208.7941390	3.9486	137.3122	-133.3637
CCSD(T)/6-311++G(d.p)	-208.7217413	-208.7187315	-208.9428752	1.1821	141.3269	-140.1448
CCSD(T)/6-311++G(df.pd)	-208.7849909	-208.7800652	-208.9971292	2.3844	136.8843	-134.5000
$d\varepsilon_{ZPE}$	4.3788	3.6722	2.9976			-1.3812
$\Delta_f H^0$(exp)[1]	146.344		18.470			-127.874

TABLE V: Total electronic energies(hartree), forward barrier($V_f + d\varepsilon_{ZPE}$), reverse barrier($V_r + d\varepsilon_{ZPE}$), and enthalpy with ZPE correction($\Delta H + d\varepsilon_{ZPE}$) and experimental heat of reaction ($\Delta_f H^0$(exp) values, given in kcal mol^{-1}, using Dunning basis set for reactant, product and TS for NF+N=N_2+F reaction.

	$NF+N$	TS	N_2+F	$V_d + d\varepsilon_{ZPE}$	$V_r + d\varepsilon_{ZPE}$	$\Delta H + d\varepsilon_{ZPE}$
MP2/cc-pVDZ	-208.5473953	-208.5395302	-208.7849231	5.2284	152.8801	-147.6517
MP2/aug-cc-pVDZ	-208.5885597	-208.5832464	-208.8230135	3.6272	149.3499	-145.7227
MP2/cc-pVTZ	-208.7518279	-208.7474655	-208.9998415	3.0305	157.2621	-154.2316
MP2/aug-cc-pVTZ	-208.7681995	-208.7666308	-209.0182104	1.2774	156.7623	-155.4849
MP4(SDQ)/cc-pVDZ	-208.5793082	-208.5731020	-208.7971118	4.1875	139.4620	-135.2746
MP4(SDQ)/aug-cc-pVDZ	-208.6222228	-208.6184019	-208.8359423	2.6907	135.4024	-132.7117
MP4(SDQ)/cc-pVTZ	-208.7813769	-208.7782546	-209.0090221	2.2523	143.7025	-141.4503
MP4(SDQ)/aug-cc-pVTZ	-208.7973493	-208.7972766	-209.0266262	0.3386	142.8128	-142.4742
MP4(SDTQ)/cc-pVDZ	-208.5868588	-208.5816755	-208.8135452	3.5456	144.3942	-140.8486
MP4(SDTQ)/aug-cc-pVDZ	-208.6332439	-208.6308825	-208.8555815	1.7748	139.8945	-138.1197
MP4(SDTQ)/cc-pVTZ	-208.7976301	-208.7962060	-209.0372541	1.1866	150.1537	-148.9671
MP4(SDTQ)/aug-cc-pVTZ	-208.8153171	-208.8171719	-209.0565876	-0.8709	149.1294	-150.0003
QCISD/cc-pVDZ	-208.5825694	-208.5839682	-208.7967257	-0.5848	132.4011	-132.9858
QCISD/aug-cc-pVDZ	-208.6257208	-208.6298276	-208.8358684	-2.2841	128.1863	-130.4703
QCISD/cc-pVTZ	-208.7839081	-208.7881518	-209.0078864	-2.3700	136.7793	-139.1492
QCISD/aug-cc-pVTZ	-208.7999687		-209.0256839			-140.2392
QCISD(T)/cc-pVDZ	-208.5886346	-208.5947290	-208.8098404	-3.5313	133.8782	-137.4095
QCISD(T)/aug-cc-pVDZ	-208.6349089	-208.6443949	-208.8518604	-5.6596	129.0803	-134.7399
QCISD(T)/cc-pVTZ	-208.7988996	-208.8090522	-209.0307763	-6.0778	138.0277	-144.1056
QCISD(T)/aug-cc-pVTZ	-208.8164346		-209.0500510			-145.1972
CCSD/cc-pVDZ	-208.5802623	-208.5816592	-208.7954798	-0.5836	133.0682	-133.6518
CCSD/aug-cc-pVDZ	-208.6229551	-208.6269505	-208.8343841	-2.2141	129.0603	-131.2744
CCSD/cc-pVTZ	-208.7814880	-208.7856447	-209.0062699	-2.3154	137.3381	-139.6535
CCSD/aug-cc-pVTZ	-208.7973815		-209.0239959			-140.8034
CCSD(T)/cc-pVDZ	-208.5877693	-208.5936903	-208.8093426	-3.4225	134.2176	-137.6401
CCSD(T)/aug-cc-pVDZ	-208.6338548	-208.6430859	-208.8513096	-5.4996	129.5561	-135.0557
CCSD(T)/cc-pVTZ	-208.7977878	-208.8076632	-209.0300555	-5.9039	138.4470	-144.3509
CCSD(T)/aug-cc-pVTZ	-208.8152480		-209.0493049			-145.4737
$d\varepsilon_{ZPE}$	1.6430	1.9360	3.0423			1.3993
$\Delta_f H^0$(exp)[1]	168.130		18.470			-149.660

TABLE VI: Total electronic energies(hartree), forward barrier($V_f + d\varepsilon_{ZPE}$), reverse barrier($V_r + d\varepsilon_{ZPE}$), and enthalpy with ZPE correction($\Delta H + d\varepsilon_{ZPE}$) and experimental heat of reaction ($\Delta_f H^0$(exp) values, given in kcal mol^{-1}, using Pople basis set for reactant, product and TS for NF+N=N_2+F reaction.

	$NF+N$	TS	N_2+F	$V_d+d\varepsilon_{ZPE}$	$V_r+d\varepsilon_{ZPE}$	$\Delta H+d\varepsilon_{ZPE}$
MP2/6-31G(d)	-208.5130611	-208.5104723	-208.7506130	1.9073	149.6217	-147.7145
MP2/6-31++G(d.p)	-208.5338765	-208.5267752	-208.7696058	4.7389	151.3097	-146.5708
MP2/6-311++G(d.p)	-208.6740535	-208.6659549	-208.9169090	5.3648	156.4072	-151.0425
MP2/6-311++G(df.pd)	-208.7219592	-208.7156711	-208.9683369	4.2287	157.4813	-153.2527
MP2/6-311++G(3df.3pd)	-208.7782746	-208.7740323	-209.0254932	2.9449	156.7253	-153.7804
MP4(SDQ)/6-31G(d)	-208.5496953	-208.5437603	-208.7611814	4.0071	135.3650	-131.3579
MP4(SDQ)/6-31++G(d.p)	-208.5655928	-208.5601613	-208.7805905	3.6911	137.2526	-133.5615
MP4(SDQ)/6-311++G(d.p)	-208.7049647	-208.6980240	-208.9269772	4.6382	142.6015	-137.9633
MP4(SDQ)/6-311++G(df.pd)	-208.7534273	-208.7489807	-208.9793326	3.0731	143.4792	-140.4061
MP4(SDQ)/6-311++G(3df.3pd)	-208.8096826	-208.8066690	-209.0360375	2.1739	142.8621	-140.6882
MP4(SDTQ)/6-31G(d)	-208.5578274	-208.5529331	-208.7791967	3.3540	140.9137	-137.5597
MP4(SDTQ)/6-31++G(d.p)	-208.5748318	-208.5705964	-208.7990214	2.9406	142.2700	-139.3295
MP4(SDTQ)/6-311++G(d.p)	-208.7163021	-208.7111632	-208.9492587	3.5075	148.3383	-144.8309
MP4(SDTQ)/6-311++G(df.pd)	-208.7665216	-208.7634858	-209.0039361	2.1878	149.8160	-147.6282
MP4(SDTQ)/6-311++G(3df.3pd)	-208.8270539	-208.8257690	-209.0653474	1.0891	149.2689	-148.1798
QCISD/6-31G(d)	-208.5531883	-208.5543882	-208.7616226	-0.4701	128.9727	-129.4429
QCISD/6-31++G(d.p)	-208.5690225	-208.5709801	-208.7805227	-0.9456	130.4211	-131.3668
QCISD/6-311++G(d.p)	-208.7084735	-208.7086445	-208.9262514	0.1755	135.4816	-135.3061
QCISD/6-311++G(df.pd)	-208.7562897	-208.7589942	-208.9783891	-1.4143	136.6035	-138.0179
QCISD(T)/6-31G(d)	-208.5591564	-208.5650043	-208.7752195	-3.3868	130.8432	-134.2300
QCISD(T)/6-31++G(d.p)	-208.5756931	-208.5825870	-208.7947996	-4.0432	132.0966	-136.1398
QCISD(T)/6-311++G(d.p)	-208.7176584	-208.7232464	-208.9436550	-3.2237	137.2396	-140.4634
QCISD(T)/6-311++G(df.pd)	-208.7678391	-208.7759745	-208.9978573	-4.8222	138.1647	-142.9870
CCSD/6-31G(d)	-208.5502674	-208.5515313	-208.7601402	-0.5103	129.8352	-130.3456
CCSD/6-31++G(d.p)	-208.5658074	-208.5677571	-208.7787244	-0.9406	131.3151	-132.2558
CCSD/6-311++G(d.p)	-208.7054011	-208.7059431	-208.9244951	-0.0573	136.0746	-136.1320
CCSD/6-311++G(df.pd)	-208.7536899	-208.7563720	-208.9767173	-1.4002	137.1999	-138.6002
CCSD(T)/6-31G(d)	-208.5581737	-208.5638684	-208.7746424	-3.2907	131.1938	-134.4846
CCSD(T)/6-31++G(d.p)	-208.5745948	-208.5812883	-208.7941390	-3.9174	132.4970	-136.4145
CCSD(T)/6-311++G(d.p)	-208.7164833	-208.7218504	-208.9428752	-3.0851	137.6263	-140.7115
CCSD(T)/6-311++G(df.pd)	-208.7666743	-208.7746066	-208.9971292	-4.6948	138.5662	-143.2610
$d\varepsilon_{ZPE}$	1.6460	1.9288	2.9976			1.3516
$\Delta_f H^0$(exp)[1]	168.130		18.470			-149.660

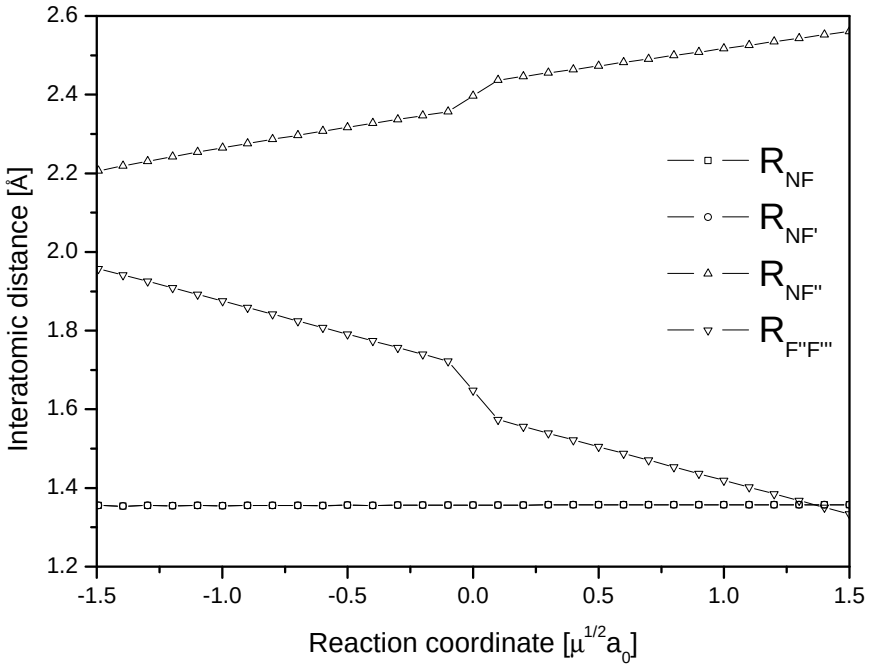

FIG. 1: IRC of the abstraction channel NF_3+F = NF_2 + F_2.

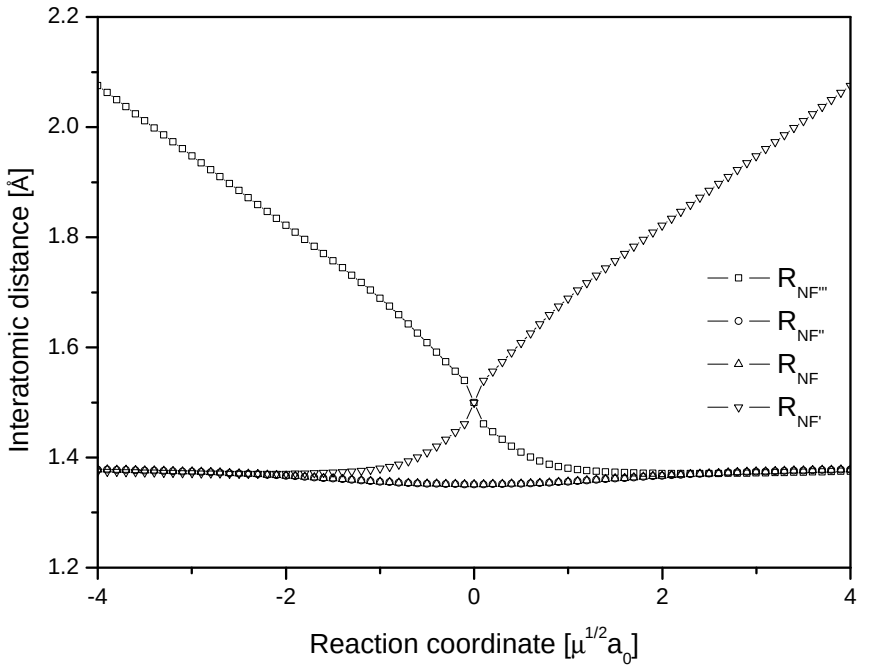

FIG. 2: IRC of the exchange channel NF_3+F = NF_3 + F.

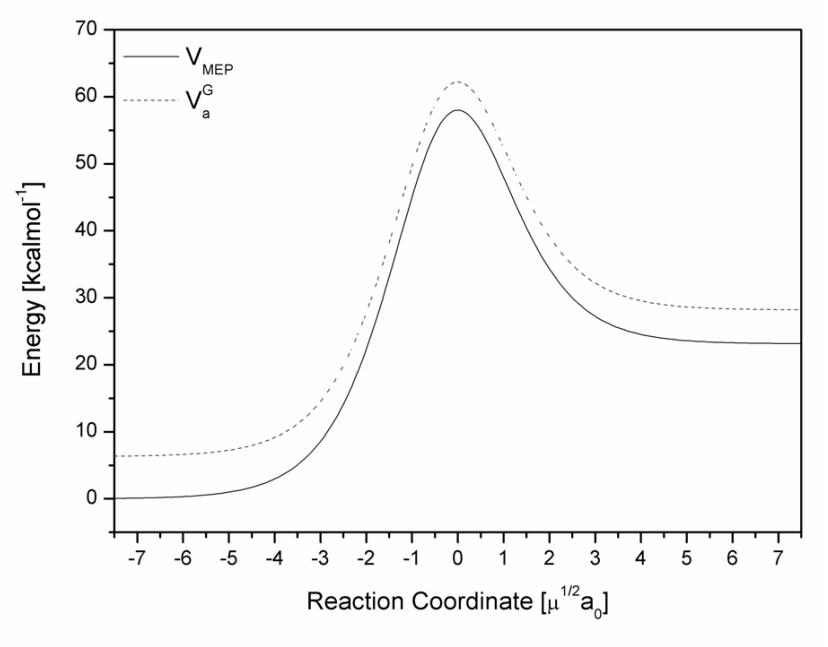

FIG. 3: MEP and $V^G{}_a$ as a function of reaction coordinate for the NF_3+F = NF_2 + F_2 abstraction reaction.

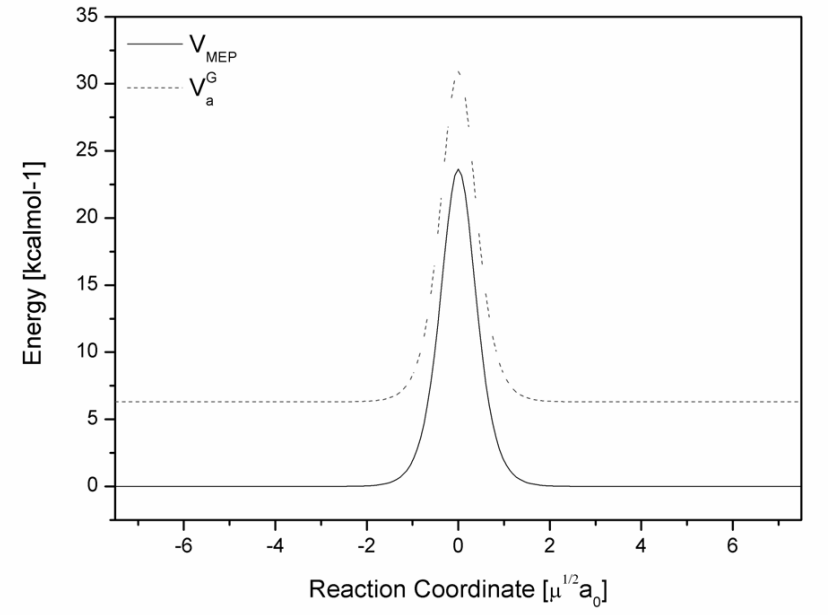

FIG. 4: MEP and $V^G{}_a$ as a function of reaction coordinate for NF_3+F = NF_3 + F exchange reaction.

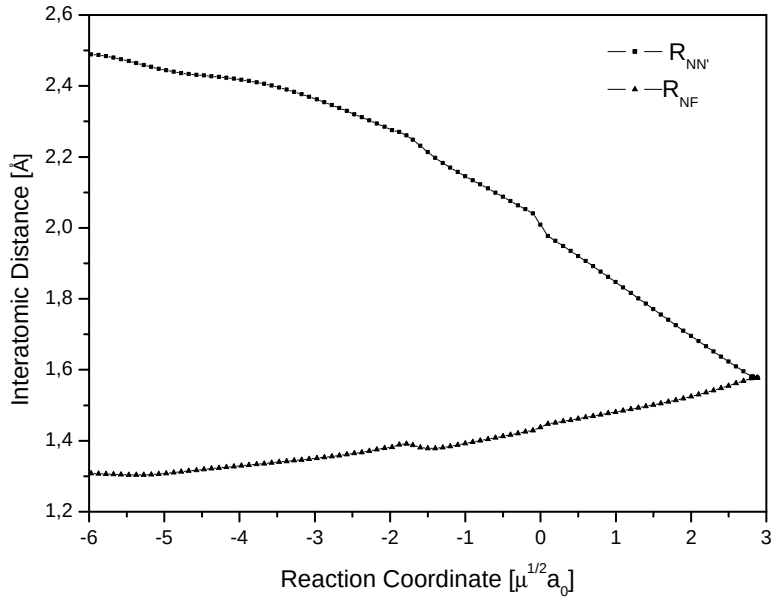

FIG. 5: IRC of the unimolecular channel $N_2F = N_2+F$.

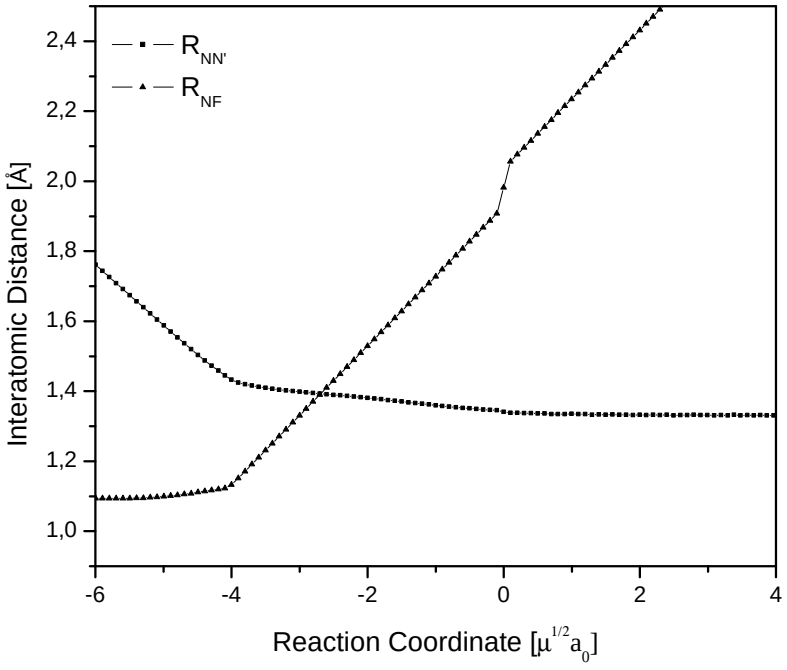

FIG. 6: IRC of the abstraction channel $NF+N = N_2+F$.

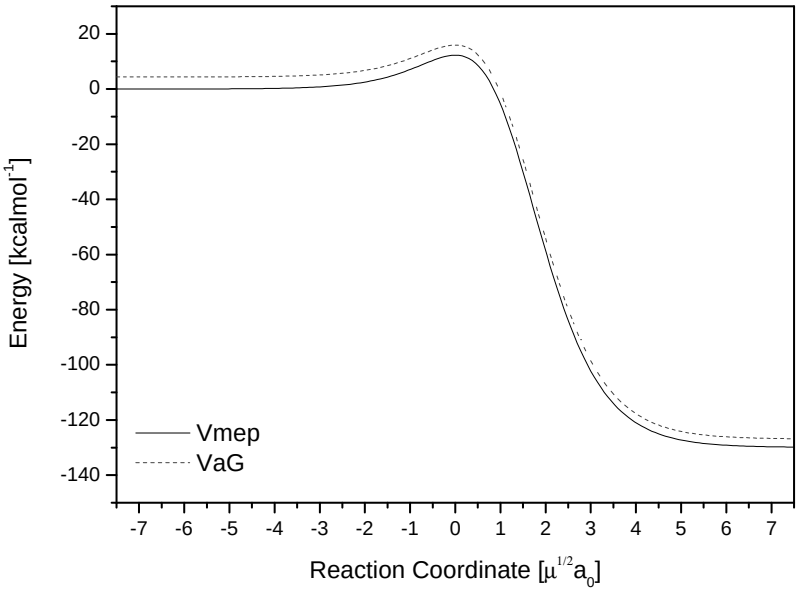

FIG. 7: MEP and $V^G{}_a$ as a function of reaction coordinate for the $N_2F = N_2 + F$ unimolecular reaction.

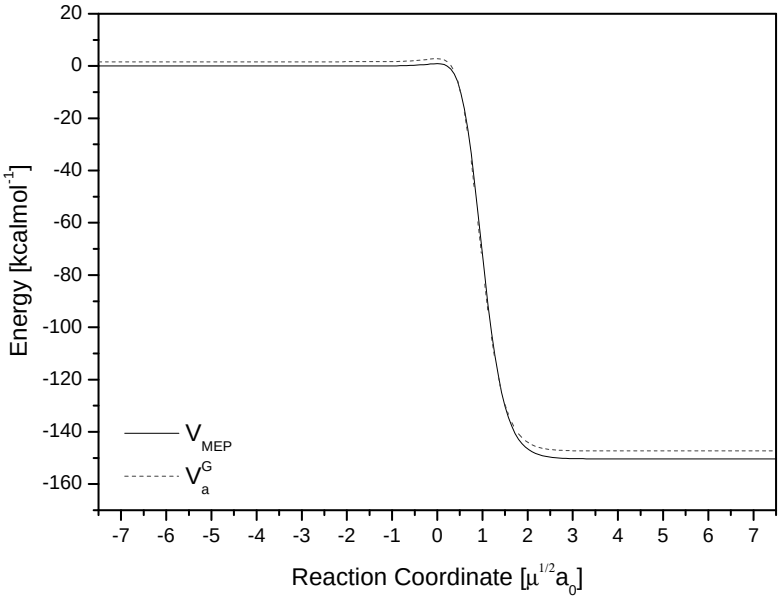

FIG. 8: MEP and $V^G{}_a$ as a function of reaction coordinate for the NF+ $N = N_2 + F$ abstraction reaction.