

Theoretical potential energy curves of the states in NO<sup>2+</sup>.

r (a.u.)	energy (Hartree)							
	<sup>6</sup> Σ <sup>+</sup>	A <sup>2</sup> Π	<sup>2</sup> Π	<sup>2</sup> Π	<sup>2</sup> Φ	X <sup>2</sup> Σ <sup>+</sup>	B <sup>2</sup> Σ <sup>+</sup>	<sup>2</sup> Δ
1.7	-127.37809	-128.10591	-127.81067	-127.66284	-127.63757	-128.29392	-128.11854	-127.69789
1.8	-127.59778	-128.21953	-127.93242	-127.77267	-127.7437	-128.37168	-128.1958	-127.84591
1.9	-127.76179	-128.2926	-128.01163	-127.85814	-127.84009	-128.41335	-128.23608	-127.94892
2	-127.88413	-128.33672	-128.06137	-127.95943	-127.91333	-128.43049	-128.25191	-128.0197
2.1	-127.97524	-128.36097	-128.09085	-128.03499	-127.99083	-128.43141	-128.25289	-128.06756
2.2	-128.04302	-128.37185	-128.10724	-128.0902	-128.04834	-128.42206	-128.24663	-128.09931
2.3	-128.09345	-128.37398	-128.13394	-128.11198	-128.09115	-128.40667	-128.23871	-128.11985
2.4	-128.13107	-128.37064	-128.16409	-128.11545	-128.12307	-128.38818	-128.23205	-128.13268
2.5	-128.15931	-128.36415	-128.18655	-128.11975	-128.14689	-128.36857	-128.22697	-128.14031
2.6	-128.18084	-128.35612	-128.20285	-128.12861	-128.16457	-128.34917	-128.22284	-128.14459
2.7	-128.19771	-128.34769	-128.21432	-128.13854	-128.17759	-128.3309	-128.21925	-128.14692
2.8	-128.21151	-128.3397	-128.22205	-128.14666	-128.18713	-128.3144	-128.21625	-128.14845
2.9	-128.2234	-128.33275	-128.22684	-128.15275	-128.19408	-128.30019	-128.21406	-128.14992
3	-128.23418	-128.32724	-128.22932	-128.15715	-128.19912	-128.28876	-128.21277	-128.15165
3.2	-128.25399	-128.32106	-128.2295	-128.16268	-128.20548	-128.27641	-128.21155	-128.15665
3.4	-128.2723	-128.32078	-128.22666	-128.16677	-128.20929	-128.27882	-128.20846	-128.16468
3.6	-128.28905	-128.32472	-128.22404	-128.17374	-128.21254	-128.28992	-128.20476	-128.17593
3.8	-128.30408	-128.33111	-128.22341	-128.18522	-128.21637	-128.30334	-128.20432	-128.18904
4	-128.31747	-128.33862	-128.22523	-128.19758	-128.2212	-128.31642	-128.20881	-128.20218
4.2	-128.32939	-128.34644	-128.22909	-128.21065	-128.22691	-128.32845	-128.21701	-128.21432
4.5	-128.34506	-128.35799	-128.23725	-128.22799	-128.23641	-128.34439	-128.2309	-128.2301
5	-128.36676	-128.37562	-128.25278	-128.25006	-128.25254	-128.36641	-128.25106	-128.25092

Theoretical potential energy curves of the states in NO<sup>2+</sup> (*continued*).

r (a.u.)	energy (Hartree)							
	C <sup>2</sup> Σ <sup>+</sup>	<sup>2</sup> Δ	<sup>2</sup> Σ <sup>-</sup>	<sup>2</sup> Δ(2)	<sup>2</sup> Δ(2)	a <sup>4</sup> Σ <sup>+</sup>	b <sup>4</sup> Δ	<sup>4</sup> Σ <sup>+</sup>
1.7	-127.7132	-127.64734	-127.70571	-127.6974	-127.64675	-127.84254	-127.78423	-127.61205
1.8	-127.86263	-127.80077	-127.85358	-127.8454	-127.80019	-127.99039	-127.93135	-127.76416
1.9	-127.96563	-127.90882	-127.95626	-127.94839	-127.90825	-128.09277	-128.03314	-127.87046
2	-128.0343	-127.98429	-128.02663	-128.01916	-127.98372	-128.16242	-128.10241	-127.94409
2.1	-128.07713	-128.03656	-128.07412	-128.06702	-128.036	-128.20869	-128.14854	-127.99482
2.2	-128.09991	-128.07251	-128.10567	-128.09878	-128.07196	-128.23841	-128.1784	-128.03
2.3	-128.1071	-128.09708	-128.12627	-128.11934	-128.09655	-128.25657	-128.19699	-128.05506
2.4	-128.10375	-128.11377	-128.13947	-128.13219	-128.11325	-128.26676	-128.2078	-128.07381
2.5	-128.09708	-128.12497	-128.14771	-128.13985	-128.12447	-128.27156	-128.21335	-128.08862
2.6	-128.09604	-128.13229	-128.15263	-128.14414	-128.13181	-128.27288	-128.21544	-128.10078
2.7	-128.10316	-128.13678	-128.15538	-128.1465	-128.13631	-128.27214	-128.21537	-128.11109
2.8	-128.11337	-128.13913	-128.15676	-128.14805	-128.13867	-128.27047	-128.21409	-128.12018
2.9	-128.12343	-128.14001	-128.15739	-128.14954	-128.13956	-128.26869	-128.21223	-128.12871
3	-128.13206	-128.14012	-128.15776	-128.15129	-128.13968	-128.26765	-128.21058	-128.13739
3.2	-128.14376	-128.14058	-128.15931	-128.15633		-128.26971	-128.20934	-128.1545
3.4	-128.15152	-128.14559	-128.16431	-128.1644	-128.14526	-128.27812	-128.21306	-128.16761
3.6	-128.16231	-128.15883	-128.17428	-128.17571	-128.1586	-128.2906	-128.22234	-128.17726
3.8	-128.17691	-128.17485	-128.18755			-128.30412	-128.23454	-128.18771
4	-128.1913	-128.18977	-128.20125			-128.31707	-128.247	-128.20217
4.2	-128.2043	-128.20294	-128.21379			-128.32896	-128.25867	-128.21543
4.5	-128.22141	-128.21981	-128.2299			-128.34475	-128.2743	-128.23075
5	-128.24348	-128.24244	-128.25087			-128.36662	-128.29611	-128.25109

Theoretical potential energy curves of the states in NO<sup>2+</sup> (*continued*).

r (a.u.)	energy (Hartree)						
	<sup>4</sup> Δ	<sup>4</sup> Π	<sup>c</sup> 4Π	<sup>b</sup> 4Δ(2)	<sup>4</sup> Σ <sup>-</sup>	<sup>4</sup> Δ(2)	<sup>4</sup> Σ <sup>-</sup>
1.7	-127.56423	-127.82263	-127.56808	-127.78417	-127.74247	-127.56418	-127.53941
1.8	-127.71713	-127.92906	-127.75816	-127.93129	-127.89021	-127.71709	-127.69233
1.9	-127.82385	-127.99366	-127.89818	-128.03309	-127.99276	-127.82381	-127.79917
2	-127.89736	-128.02893	-128.00145	-128.10236	-128.06293	-127.89732	-127.87279
2.1	-127.94743	-128.07785	-128.04399	-128.14848	-128.11012	-127.9474	-127.92277
2.2	-127.98212	-128.13437	-128.04615	-128.17835	-128.14121	-127.98211	-127.95648
2.3	-128.00914	-128.17637	-128.04099	-128.19695	-128.16121	-128.00918	-127.97997
2.4	-128.03452	-128.20768	-128.03353	-128.20777	-128.17358	-128.0346	-127.99824
2.5	-128.05804	-128.23107	-128.02857	-128.21333	-128.1808	-128.05814	-128.0144
2.6	-128.078	-128.24858	-128.02965	-128.21542	-128.18463	-128.07812	-128.0292
2.7	-128.09457	-128.26172	-128.03711	-128.21537	-128.18633	-128.0947	-128.04285
2.8	-128.10863	-128.27166	-128.04972	-128.21411	-128.18683	-128.10876	-128.05706
2.9	-128.12087	-128.27908	-128.08583	-128.21224	-128.18672	-128.12097	-128.08641
3	-128.13223	-128.2851	-128.11396	-128.21061	-128.18723	-128.13232	-128.11397
3.2	-128.153	-128.29453	-128.16028	-128.20941	-128.19257	-128.15307	-128.14944
3.4	-128.1702	-128.30293	-128.19521	-128.21318	-128.20768	-128.17024	-128.16668
3.6	-128.18309	-128.31195	-128.22105	-128.22252	-128.22698	-128.18311	-128.1771
3.8	-128.19393	-128.32184	-128.24037	-128.23476	-128.24469	-128.19397	-128.1899
4	-128.20485	-128.33203	-128.25551	-128.24724	-128.25971	-128.20492	-128.20382
4.2	-128.21581	-128.34193	-128.268	-128.25892	-128.27231	-128.21584	-128.21584
4.5	-128.23077	-128.35556	-128.28355	-128.27457	-128.28779	-128.23078	-128.23101
5	-128.25109	-128.37486	-128.30409	-128.29638	-128.30769	-128.25109	-128.25119