Cartesian coordinates for the optimized structures at the B3LYP/6-311++G(d,p) level of theory

TA2-R^+

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	0.673541	-1.648321	0.830624
2	N	-0.624924	-1.776481	0.263117
3	C	-1.060404	-1.095550	-0.803908
4	C	-0.269788	-0.129988	-1.431680
5	C	1.152980	-0.012986	-0.991147
6	O	1.959872	0.701716	-1.531797
7	O	0.980452	-2.253986	1.820206
8	N	1.487878	-0.786619	0.126697
9	C	-0.643278	0.447668	-2.756566
10	H	-1.216939	-2.457334	0.728023
11	H	-2.065367	-1.317255	-1.144959
12	H	2.444882	-0.711785	0.458943
13	H	-0.171823	1.418051	-2.907581
14	H	-1.724523	0.532163	-2.873055
15	H	-0.266374	-0.206084	-3.552694
16	N	-0.827053	1.750336	-0.073519
17	H	-1.776407	2.019820	-0.314574
18	H	-0.168778	2.427829	-0.449785
19	H	-0.711955	1.641840	0.956056
20	N	-0.512026	1.622135	2.888422
21	H	-1.403400	1.801625	3.346349
22	H	0.096359	2.395411	3.150562
23	H	-0.124749	0.796078	3.339966

TA2-5I^{+}*

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-2.532512	-0.094067	-1.296102
2	N	-1.513858	-0.386864	-2.222695
3	C	-0.970141	-1.610965	-2.411024
4	C	-1.255029	-2.683564	-1.530662
5	C	-2.471767	-2.503132	-0.645802
6	O	-2.945409	-3.404160	0.000521
7	O	-2.965420	1.017943	-1.151651
8	N	-2.972908	-1.207589	-0.593485
9	C	-0.998225	-4.088653	-2.011536
10	N	0.058619	-2.571379	-0.035163
11	H	-1.258188	0.391768	-2.819983
12	H	-0.266502	-1.712589	-3.227479
13	H	-0.473500	0.723199	1.200024
14	H	-3.765578	-1.051231	0.022131
15	H	-1.088926	-4.806336	-1.197449
16	H	-0.015981	-4.176865	-2.479418
17	H	-1.752862	-4.353689	-2.758156
18	H	0.980003	-2.761474	-0.423585
19	H	-0.200127	-3.323066	0.602599
20	N	0.103859	-0.064207	1.489407
21	H	-0.174768	-0.275773	2.446084
22	H	1.054799	0.295189	1.551060
23	H	0.052748	-1.648157	0.466605

TA2-5I^{+}

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-3.098224	-0.529344	-1.926268
2	N	-1.796252	-0.473298	-2.393786
3	C	-0.719365	-1.165663	-1.877497
4	C	-1.026514	-2.400903	-1.094820
5	C	-2.339102	-2.246148	-0.292719
6	O	-2.494051	-2.860096	0.741985
7	O	-4.000190	0.136405	-2.362598
8	N	-3.278867	-1.432445	-0.855665
9	C	-1.123751	-3.672999	-1.970534
10	N	0.025107	-2.635996	-0.029348
11	H	-1.653269	0.210719	-3.126577
12	H	0.216522	-1.063569	-2.411601
13	H	0.673077	0.471250	1.027413
14	H	-4.195108	-1.402100	-0.418563
15	H	-1.361424	-4.552612	-1.366775
16	H	-0.182892	-3.838820	-2.502221
17	H	-1.909437	-3.547488	-2.716716
18	H	0.875511	-3.036209	-0.428339
19	H	-0.377195	-3.304919	0.641281
20	N	0.640927	-0.412938	1.531666
21	H	-0.060216	-0.300848	2.262738
22	H	1.536373	-0.501622	2.009707
23	H	0.276668	-1.736015	0.533483

TA2-5P*$^{+}$

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-3.067977	-0.562762	-2.043854
2	N	-1.823533	-0.607721	-2.646678
3	C	-0.699777	-1.209118	-2.116276
4	C	-0.931666	-2.310155	-1.127393
5	C	-2.105902	-1.934885	-0.201392
6	O	-2.125530	-2.271811	0.966667
7	O	-4.020729	0.015705	-2.498948
8	N	-3.116920	-1.235868	-0.803141
9	C	-1.252945	-3.664364	-1.812681
10	N	0.269967	-2.457744	-0.239750
11	H	-1.757069	-0.062897	-3.497351
12	H	0.186762	-1.198212	-2.737633
13	H	0.350097	0.239936	1.461797
14	H	-3.968602	-1.089303	-0.270490
15	H	-1.478276	-4.434439	-1.069501
16	H	-0.401863	-3.987072	-2.417518
17	H	-2.116279	-3.562764	-2.471901
18	H	1.115372	-2.498064	-0.808817
19	H	0.202715	-3.349845	0.252663
20	N	0.357777	-0.743227	1.730745
21	H	-0.499533	-0.939291	2.250191
22	H	1.151022	-0.888066	2.354560
23	H	0.361215	-1.543685	0.720945

TA2-5P^{+}

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-3.410533	2.831664	1.233223
2	N	-2.341081	3.693278	1.141393
3	C	-1.021289	3.305938	1.027937
4	C	-0.706652	1.942949	0.482255
5	C	-1.809461	0.939045	0.893710
6	O	-1.621064	-0.269772	0.941786
7	O	-4.555925	3.167253	1.398220
8	N	-3.040810	1.468806	1.134600
9	C	-0.640433	1.943299	-1.067912
10	N	0.605436	1.454632	1.001628
11	H	-2.575822	4.666917	1.289269
12	H	-0.291623	4.101199	0.956138
13	H	-0.163957	-1.455919	0.812330
14	H	-3.799141	0.814331	1.299703
15	H	-0.434233	0.942532	-1.455139
16	H	0.146401	2.624363	-1.402856
17	H	-1.583712	2.289119	-1.492968
18	H	1.345957	1.991723	0.552712
19	H	0.668326	1.680252	1.995044
20	N	0.862684	-1.337310	0.817775
21	H	1.272999	-1.781851	1.639161
22	H	0.947892	-0.264042	0.857801
23	H	1.282135	-1.726173	-0.026590

TA2-6I*$^{+}$

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	0.641733	-1.374586	0.899748
2	N	-0.670481	-1.290756	0.376468
3	C	-1.028171	-0.522609	-0.676753
4	C	-0.010463	-0.101420	-1.595585
5	C	1.398458	-0.237293	-1.184344
6	O	2.324727	0.151702	-1.860159
7	O	0.857165	-1.880722	1.968612
8	N	1.600113	-0.832220	0.069117
9	C	-0.324679	0.494812	-2.914048
10	H	-1.373477	-1.731927	0.957630
11	H	-2.036310	-0.666655	-1.042434
12	H	2.562208	-0.919988	0.381747
13	H	0.246798	1.414944	-3.072161
14	H	-1.390508	0.686090	-3.041454
15	H	0.002663	-0.183485	-3.713583
16	N	-1.570522	1.344628	0.139876
17	H	-2.584182	1.394576	0.225303
18	H	-1.258406	2.139905	-0.413523
19	H	-1.132960	1.379251	1.091250
20	N	-0.363407	1.441058	2.845664
21	H	-1.068170	1.750643	3.512417
22	H	0.387402	2.126844	2.900031
23	H	0.018651	0.575500	3.223871

TA2-6I^{+}

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-1.071406	1.020354	-1.849031
2	N	0.013272	1.648983	-1.234468
3	C	0.864889	1.059929	-0.267864
4	C	0.920983	-0.432732	-0.357886
5	C	-0.209770	-1.142811	-0.953317
6	O	-0.327379	-2.353375	-0.918986
7	O	-1.836030	1.609120	-2.567930
8	N	-1.188124	-0.333535	-1.545534
9	C	2.098790	-1.183815	0.143092
10	N	0.362209	1.450733	1.179683
11	H	0.183519	2.590974	-1.560428
12	H	1.864568	1.495011	-0.326048
13	H	-1.938432	-0.818619	-2.026531
14	H	1.853881	-2.238346	0.266441
15	H	2.487471	-0.786644	1.087860
16	H	2.925973	-1.118552	-0.579501
17	H	0.987288	1.074210	1.896500
18	H	0.357815	2.468865	1.279103
19	H	-0.652278	1.083407	1.377483
20	N	-2.204620	0.547444	1.740450
21	H	-2.496682	0.795933	2.684703
22	H	-2.304780	-0.464363	1.670383
23	H	-2.904000	0.944759	1.114508

TA2-6P*$^{+}$

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-1.239238	0.794177	-1.479064
2	N	-0.114657	1.488132	-1.057742
3	C	0.828154	0.940541	-0.130926
4	C	1.090967	-0.511060	-0.409180
5	C	0.029388	-1.303757	-1.016472
6	O	0.088698	-2.507900	-1.175916
7	O	-2.242486	1.347815	-1.876746
8	N	-1.128362	-0.583880	-1.370609
9	C	2.400283	-1.126210	-0.080404
10	N	0.291627	1.108441	1.315934
11	H	-0.165350	2.488789	-1.194523
12	H	1.757694	1.509117	-0.186503
13	H	-1.882020	-1.120208	-1.787013
14	H	2.331550	-2.213023	-0.110287
15	H	2.777509	-0.809348	0.898825
16	H	3.159675	-0.818750	-0.814597
17	H	0.670739	0.381814	1.925410
18	H	0.613586	1.999524	1.698258
19	H	-1.002375	1.112148	1.374162
20	N	-2.337761	1.172668	1.425163
21	H	-2.663330	1.841704	2.122781
22	H	-2.749961	0.269818	1.660581
23	H	-2.727174	1.456379	0.521550

TA2-6P^{+}

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	-1.285263	0.572059	-1.214039
2	N	-0.200438	1.343038	-0.883003
3	C	0.832709	0.813111	-0.006174
4	C	1.241176	-0.551871	-0.489374
5	C	0.242220	-1.381511	-1.141316
6	O	0.409478	-2.541514	-1.466741
7	O	-2.418674	1.045994	-1.345084
8	N	-1.022964	-0.765960	-1.333332
9	C	2.621451	-1.054472	-0.281542
10	N	0.328363	0.786897	1.414608
11	H	-0.378068	2.337924	-0.865711
12	H	1.684582	1.492855	-0.053231
13	H	-1.771843	-1.355180	-1.679321
14	H	2.676675	-2.125077	-0.474300
15	H	2.982262	-0.846350	0.731878
16	H	3.317188	-0.550815	-0.968065
17	H	0.323129	-0.165147	1.776606
18	H	0.949299	1.315591	2.022883
19	H	-1.556091	1.436855	1.500179
20	N	-2.555373	1.715789	1.311022
21	H	-2.715928	2.683904	1.593599
22	H	-3.194481	1.110966	1.829977
23	H	-2.722251	1.599849	0.273167

TA1-R^+

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	1.258292	-0.679388	-1.527920
2	N	1.933122	-0.804645	-0.269108
3	C	1.341014	-0.754065	0.921828
4	C	-0.035846	-0.529116	1.046059
5	C	-0.839515	-0.416372	-0.206466
6	O	-2.034526	-0.260237	-0.211532
7	O	1.871114	-0.736888	-2.554202
8	N	-0.099695	-0.495883	-1.393363
9	C	-0.751506	-0.685381	2.336752
10	N	0.082150	2.054028	1.114230
11	H	2.933293	-0.967163	-0.352654
12	H	1.974521	-0.893734	1.791023
13	H	-0.625288	-0.429741	-2.261021
14	H	-1.642002	-0.057552	2.367902
15	H	-0.106743	-0.482841	3.192478
16	H	-1.109058	-1.721426	2.421547
17	H	0.297655	2.330194	2.068370
18	H	-0.890149	2.279734	0.917644
19	H	0.677192	2.579336	0.478833

TA1-5I*$^{+}$

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	1.266294	-0.811063	-1.512264
2	N	1.961749	-0.721536	-0.300702
3	C	1.391253	-0.506807	0.918862
4	C	0.028244	-0.053194	1.030201
5	C	-0.790742	-0.134428	-0.266882
6	O	-1.956373	0.182117	-0.282319
7	O	1.795788	-1.090292	-2.551897
8	N	-0.101213	-0.536096	-1.388781
9	C	-0.729661	-0.544567	2.252950
10	N	-0.028916	1.712097	1.252850
11	H	2.935981	-0.995954	-0.365355
12	H	2.014088	-0.666117	1.788660
13	H	-0.633361	-0.599888	-2.252661
14	H	-1.712503	-0.078190	2.324947
15	H	-0.161046	-0.362948	3.168057
16	H	-0.883011	-1.622387	2.163816
17	H	0.315019	1.953565	2.182978
18	H	-1.007540	1.999395	1.163031
19	H	0.529973	2.205153	0.554909

TA1-5I^{+}

Center Number	Atom	Coordinates (Å)		
		x	y	z
1	C	1.095591	-1.195311	-1.323479
2	N	1.891113	-0.841340	-0.244313
3	C	1.546521	0.014872	0.778358
4	C	0.092087	0.266141	0.983663
5	C	-0.684464	0.237973	-0.356655
6	O	-1.682553	0.919028	-0.477734
7	O	1.452972	-1.915314	-2.214952
8	N	-0.189988	-0.603565	-1.301988
9	C	-0.586049	-0.685697	1.993018
10	N	-0.146775	1.700428	1.476849
11	H	2.830666	-1.218337	-0.287820
12	H	2.249531	0.092775	1.598000
13	H	-0.734174	-0.730778	-2.150973
14	H	-1.646898	-0.451295	2.114594
15	H	-0.082771	-0.634116	2.962341
16	H	-0.503785	-1.711596	1.631759
17	H	-0.114701	1.775333	2.496212
18	H	-1.090065	1.960151	1.128755
19	H	0.537768	2.349506	1.074765