Electronic Supporting Information for 'On the Unprecedented Level of Dinitrogen Activation in the Calix[4]arene Complex of Nb(III)'

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1 Notes

In Cartesian coordinate records, Xx denotes a 'dummy atom' (*i.e.*, an atom that does not take part in the electronic structure calculation, but which prevents poorly-defined angles in the Z-matrix representation of the molecule.)

Geometries are presented in a two-column layout proceeding from left to right, and are terminated with a single black horizontal line.

Some geometries given are recalculations that may not be perfectly isostructural with those given in the main paper but are otherwise negligibly discrepant.

2 Standard geometries

2.1 ADF software geometry optimisation, complex (1), D_{4h} symmetry

Table 1: Cartesian coordinates of **(1)** in D_{4h} Symmetry GGA Becke Perdew / TZP-ZORA, spin singlet. Equilibrium N−N distance 1.260 Å

Atom	X	Y	Z
Xx	-1.000000	0.000000	0.700000
N	0.000000	0.000000	0.630098
Nb	0.000000	0.000000	2.457700
O	-1.988943	0.000000	2.903922
O	0.000000	-1.988943	2.903922
O	1.988943	0.000000	2.903922
O	0.000000	1.988943	2.903922
C	-2.641684	0.000000	4.078736
C	-3.014834	1.224493	4.691064
C	-3.783456	1.195884	5.859462
C	-4.195577	0.000000	6.470467
C	-3.783456	-1.195884	5.859462
C	-3.014834	-1.224493	4.691064
C	2.641684	0.000000	4.078736
C	3.014834	-1.224493	4.691064
C	3.783456	-1.195884	5.859462
C	4.195577	0.000000	6.470467
C	3.783456	1.195884	5.859462
C	3.014834	1.224493	4.691064
C	0.000000	-2.641684	4.078736
C	-1.224493	-3.014834	4.691064
C	-1.195884	-3.783456	5.859462
C	0.000000	-4.195577	6.470467
C	1.195884	-3.783456	5.859462
C	1.224493	-3.014834	4.691064
C	0.000000	2.641684	4.078736
C	1.224493	3.014834	4.691064
C	1.195884	3.783456	5.859462
C	0.000000	4.195577	6.470467
C	-1.195884	3.783456	5.859462
C	-1.224493	3.014834	4.691064
C	-2.545499	-2.545499	4.101500
C	2.545499	-2.545499	4.101500
C	2.545499	2.545499	4.101500
C	-2.545499	2.545499	4.101500
H	-3.311959	-3.311959	4.290833
H	-2.430675	-2.430675	3.017504
H	3.311959	3.311959	4.290833
H	2.430675	2.430675	3.017504
H	3.311959	-3.311959	4.290833

H	2.430675	-2.430675	3.017504
H	-3.311959	3.311959	4.290833
H	-2.430675	2.430675	3.017504
H	-4.059108	2.156034	6.300336
H	-4.059108	-2.156034	6.300336
C	-4.962841	0.000000	7.805973
H	4.059108	-2.156034	6.300336
H	4.059108	2.156034	6.300336
C	4.962841	0.000000	7.805973
H	-2.156034	-4.059108	6.300336
H	2.156034	-4.059108	6.300336
C	0.000000	-4.962841	7.805973
H	2.156034	4.059108	6.300336
H	-2.156034	4.059108	6.300336
C	0.000000	4.962841	7.805973
C	-5.865185	-1.244902	7.945033
C	-3.940963	0.000000	8.969168
C	-5.865185	1.244902	7.945033
H	-6.438610	-1.191888	8.884821
H	-4.453312	0.000000	9.947560
H	-6.438610	1.191888	8.884821
H	-6.575710	-1.315199	7.108325
H	-5.280880	-2.174455	7.970360
H	-3.291963	-0.885669	8.914653
H	-3.291963	0.885669	8.914653
H	-5.280880	2.174455	7.970360
H	-6.575710	1.315199	7.108325
C	5.865185	1.244902	7.945033
C	3.940963	0.000000	8.969168
C	5.865185	-1.244902	7.945033
H	6.438610	1.191888	8.884821
H	4.453312	0.000000	9.947560
H	6.438610	-1.191888	8.884821
H	6.575710	1.315199	7.108325
H	5.280880	2.174455	7.970360
H	3.291963	0.885669	8.914653
H	3.291963	-0.885669	8.914653
H	5.280880	-2.174455	7.970360
H	6.575710	-1.315199	7.108325
C	1.244902	-5.865185	7.945033
C	0.000000	-3.940963	8.969168
C	-1.244902	-5.865185	7.945033
H	1.191888	-6.438610	8.884821
H	0.000000	-4.453312	9.947560
H	-1.191888	-6.438610	8.884821
H	1.315199	-6.575710	7.108325
H	2.174455	-5.280880	7.970360
H	0.885669	-3.291963	8.914653
H	-0.885669	-3.291963	8.914653
H	-2.174455	-5.280880	7.970360
H	-1.315199	-6.575710	7.108325
C	-1.244902	5.865185	7.945033
C	0.000000	3.940963	8.969168
C	1.244902	5.865185	7.945033
H	-1.191888	6.438610	8.884821
H	0.000000	4.453312	9.947560
H	1.191888	6.438610	8.884821
H	-1.315199	6.575710	7.108325
H	-2.174455	5.280880	7.970360
H	-0.885669	3.291963	8.914653
H	0.885669	3.291963	8.914653
H	2.174455	5.280880	7.970360
H	1.315199	6.575710	7.108325
N	0.000000	0.000000	-0.630098
Xx	1.000000	0.000000	-0.700000
Nb	0.000000	0.000000	-2.457700
O	1.988943	0.000000	-2.903922
O	0.000000	-1.988943	-2.903922
O	-1.988943	0.000000	-2.903922
O	0.000000	1.988943	-2.903922
C	2.641684	0.000000	-4.078736
C	3.014834	1.224493	-4.691064
C	3.783456	1.195884	-5.859462
C	4.195577	0.000000	-6.470467
C	3.783456	-1.195884	-5.859462
C	3.014834	-1.224493	-4.691064
C	-2.641684	0.000000	-4.078736
C	-3.014834	-1.224493	-4.691064
C	-3.783456	-1.195884	-5.859462
C	-4.195577	0.000000	-6.470467
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C	0.000000	-2.641684	-4.078736
C	1.224493	-3.014834	-4.691064
C	1.195884	-3.783456	-5.859462
C	0.000000	-4.195577	-6.470467
C	-1.195884	-3.783456	-5.859462
C	-1.224493	-3.014834	-4.691064

C	0.000000	2.641684	-4.078736
C	-1.224493	3.014834	-4.691064
C	-1.195884	3.783456	-5.859462
C	0.000000	4.195577	-6.470467
C	1.195884	3.783456	-5.859462
C	1.224493	3.014834	-4.691064
C	2.545499	-2.545499	-4.101500
C	-2.545499	-2.545499	-4.101500
C	-2.545499	2.545499	-4.101500
C	2.545499	2.545499	-4.101500
H	3.311959	-3.311959	-4.290833
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H	-3.311959	3.311959	-4.290833
H	-2.430675	2.430675	-3.017504
H	-3.311959	-3.311959	-4.290833
H	-2.430675	-2.430675	-3.017504
H	3.311959	3.311959	-4.290833
H	2.430675	2.430675	-3.017504
H	4.059108	2.156034	-6.300336
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H	-2.156034	-4.059108	-6.300336
H	-2.156034	4.059108	-6.300336
H	2.156034	4.059108	-6.300336
C	4.962841	0.000000	-7.805973
C	5.865185	-1.244902	-7.945033
C	3.940963	0.000000	-8.969168
C	5.865185	1.244902	-7.945033
C	-4.962841	0.000000	-7.805973
C	-5.865185	1.244902	-7.945033
C	-3.940963	0.000000	-8.969168
C	-5.865185	-1.244902	-7.945033
C	0.000000	-4.962841	-7.805973
C	-1.244902	-5.865185	-7.945033
C	0.000000	-3.940963	-8.969168
C	1.244902	-5.865185	-7.945033
C	0.000000	4.962841	-7.805973
C	1.244902	5.865185	-7.945033
C	0.000000	3.940963	-8.969168
C	-1.244902	5.865185	-7.945033
H	6.438610	-1.191888	-8.884821
H	4.453312	0.000000	-9.947560
H	6.438610	1.191888	-8.884821
H	6.575710	-1.315199	-7.108325
H	5.280880	-2.174455	-7.970360
H	3.291963	-0.885669	-8.914653
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H	-4.453312	0.000000	-9.947560
H	-6.438610	-1.191888	-8.884821
H	-6.575710	1.315199	-7.108325
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H	-3.291963	-0.885669	-8.914653
H	-5.280880	-2.174455	-7.970360
H	-6.575710	-1.315199	-7.108325
H	-1.191888	-6.438610	-8.884821
H	0.000000	-4.453312	-9.947560
H	1.191888	-6.438610	-8.884821
H	-1.315199	-6.575710	-7.108325
H	-2.174455	-5.280880	-7.970360
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H	0.885669	-3.291963	-8.914653
H	2.174455	-5.280880	-7.970360
H	1.315199	-6.575710	-7.108325
H	1.191888	6.438610	-8.884821
H	0.000000	4.453312	-9.947560
H	-1.191888	6.438610	-8.884821
H	1.315199	6.575710	-7.108325
H	2.174455	5.280880	-7.970360
H	0.885669	3.291963	-8.914653
H	-0.885669	3.291963	-8.914653
H	-2.174455	5.280880	-7.970360
H	-1.315199	6.575710	-7.108325

2.2 ADF software geometry optimisation, complex (1), D_{4d} symmetry

Table 2: Cartesian coordinates of **(1)** in D_{4d} Symmetry GGA Becke Perdew / TZP-ZORA, spin singlet. Equilibrium N−N distance 1.262 Å

Atom	X	Y	Z
C	-2.283629	2.314768	4.691462
C	-1.009757	2.437770	4.079028
C	-0.022018	3.251558	4.691462
C	-0.342187	3.950363	5.860363
C	-1.604078	3.872587	6.472288

C	-2.551365	3.035291	5.860363
O	-0.760300	1.835527	2.903402
Nb	0.000000	0.000000	2.456936
O	1.835527	0.760300	2.903402
C	2.437770	1.009757	4.079028
C	3.251558	0.022018	4.691462
C	3.950363	0.342187	5.860363
C	3.872587	1.604078	6.472288
C	3.035291	2.551365	5.860363
C	2.314768	2.283629	4.691462
C	3.325166	-1.377329	4.101276
C	2.283629	-2.314768	4.691462
C	1.009757	-2.437770	4.079028
C	0.022018	-3.251558	4.691462
C	0.342187	-3.950363	5.860363
C	1.604078	-3.872587	6.472288
C	2.551365	-3.035291	5.860363
C	4.580439	1.897280	7.809265
C	5.890313	1.092262	7.949024
C	1.377329	3.325166	4.101276
O	0.760300	-1.835527	2.903402
C	-1.377329	-3.325166	4.101276
C	-2.314768	-2.283629	4.691462
C	-2.437770	-1.009757	4.079028
C	-3.251558	-0.022018	4.691462
C	-3.950363	-0.342187	5.860363
C	-3.872587	-1.604078	6.472288
C	-3.035291	-2.551365	5.860363
O	-1.835527	-0.760300	2.903402
C	-3.325166	1.377329	4.101276
C	-4.580439	-1.897280	7.809265
C	-5.890313	-1.092262	7.949024
C	1.897280	-4.580439	7.809265
C	1.092262	-5.890313	7.949024
C	-1.897280	4.580439	7.809265
C	-1.092262	5.890313	7.949024
N	0.000000	0.000000	0.631238
Xx	-0.923910	-0.382643	0.694993
N	0.000000	0.000000	-0.631238
Xx	-0.923900	0.382715	-0.695012
Nb	0.000000	0.000000	-2.456936
O	0.760300	1.835527	-2.903402
C	1.009757	2.437770	-4.079028
C	0.022018	3.251558	-4.691462
C	0.342187	3.950363	-5.860363
C	1.604078	3.872587	-6.472288
C	2.551365	3.035291	-5.860363
C	2.283629	2.314768	-4.691462
C	-1.377329	3.325166	-4.101276
C	-2.314768	2.283629	-4.691462
C	-2.437770	1.009757	-4.079028
C	-3.251558	0.022018	-4.691462
C	-3.950363	0.342187	-5.860363
C	-3.872587	1.604078	-6.472288
C	-3.035291	2.551365	-5.860363
O	-1.835527	0.760300	-2.903402
C	-3.325166	-1.377329	-4.101276
C	-2.283629	-2.314768	-4.691462
C	-1.009757	-2.437770	-4.079028
C	-0.022018	-3.251558	-4.691462
C	-0.342187	-3.950363	-5.860363
C	-1.604078	-3.872587	-6.472288
C	-2.551365	-3.035291	-5.860363
C	-4.580439	1.897280	-7.809265
C	-5.890313	1.092262	-7.949024
O	-0.760300	-1.835527	-2.903402
C	1.377329	-3.325166	-4.101276
C	2.314768	-2.283629	-4.691462
C	2.437770	-1.009757	-4.079028
C	3.251558	-0.022018	-4.691462
C	3.950363	-0.342187	-5.860363
C	3.872587	-1.604078	-6.472288
C	3.035291	-2.551365	-5.860363
O	1.835527	-0.760300	-2.903402
C	3.325166	1.377329	-4.101276
C	4.580439	-1.897280	-7.809265
C	5.890313	-1.092262	-7.949024
C	-1.897280	-4.580439	-7.809265
C	-1.092262	-5.890313	-7.949024
C	1.897280	4.580439	-7.809265
C	1.092262	5.890313	-7.949024
C	4.937426	-3.392735	-7.949024
C	3.635403	-1.505833	-8.971605
C	-4.937426	3.392735	-7.949024
C	-3.635403	1.505833	-8.971605
C	-3.392735	-4.937426	-7.949024
C	-1.505833	-3.635403	-8.971605
C	3.392735	4.937426	-7.949024

C	1.505833	3.635403	-8.971605
C	-4.937426	-3.392735	7.949024
C	-3.635403	-1.505833	8.971605
C	4.937426	3.392735	7.949024
C	3.635403	1.505833	8.971605
C	3.392735	-4.937426	7.949024
C	1.505833	-3.635403	8.971605
C	-3.392735	4.937426	7.949024
C	-1.505833	3.635403	8.971605
H	1.791951	-4.326152	-4.291658
H	1.315686	-3.176347	-3.017180
H	-1.791951	4.326152	-4.291658
H	-1.315686	3.176347	-3.017180
H	-4.326152	-1.791951	-4.291658
H	-3.176347	-1.315686	-3.017180
H	4.326152	1.791951	-4.291658
H	3.176347	1.315686	-3.017180
H	4.571981	0.439789	-6.301293
H	2.921901	-3.543856	-6.301293
H	-4.571981	-0.439789	-6.301293
H	-2.921901	3.543856	-6.301293
H	0.439789	-4.571981	-6.301293
H	-3.543856	-2.921901	-6.301293
H	-0.439789	4.571981	-6.301293
H	3.543856	2.921901	-6.301293
H	5.486221	-3.563102	-8.889578
H	4.108256	-1.701696	-9.950306
H	6.398837	-1.359850	-8.889578
H	5.567801	-3.729851	-7.113149
H	4.041456	-4.027455	-7.973429
H	2.697108	-2.075892	-8.916551
H	3.375021	-0.439266	-8.916551
H	5.705582	-0.009900	-7.973429
H	6.574433	-1.299627	-7.113149
H	-5.486221	3.563102	-8.889578
H	-4.108256	1.701696	-9.950306
H	-6.398837	1.359850	-8.889578
H	-5.567801	3.729851	-7.113149
H	-4.041456	4.027455	-7.973429
H	-2.697108	2.075892	-8.916551
H	-3.375021	0.439266	-8.916551
H	-5.705582	0.009900	-7.973429
H	-6.574433	1.299627	-7.113149
H	-3.563102	-5.486221	-8.889578
H	-1.701696	-4.108256	-9.950306
H	-1.359850	-6.398837	-8.889578
H	-3.729851	-5.567801	-7.113149
H	-4.027455	-4.041456	-7.973429
H	-2.075892	-2.697108	-8.916551
H	-0.439266	-3.375021	-8.916551
H	-0.009900	-5.705582	-7.973429
H	-1.299627	-6.574433	-7.113149
H	3.563102	5.486221	-8.889578
H	1.701696	4.108256	-9.950306
H	1.359850	6.398837	-8.889578
H	3.729851	5.567801	-7.113149
H	4.027455	4.041456	-7.973429
H	2.075892	2.697108	-8.916551
H	0.439266	3.375021	-8.916551
H	0.009900	5.705582	-7.973429
H	1.299627	6.574433	-7.113149
H	-1.791951	-4.326152	4.291658
H	-1.315686	-3.176347	3.017180
H	1.791951	4.326152	4.291658
H	1.315686	3.176347	3.017180
H	4.326152	-1.791951	4.291658
H	3.176347	-1.315686	3.017180
H	-4.326152	1.791951	4.291658
H	-3.176347	1.315686	3.017180
H	-4.571981	0.439789	6.301293
H	-2.921901	-3.543856	6.301293
H	4.571981	-0.439789	6.301293
H	2.921901	3.543856	6.301293
H	-0.439789	-4.571981	6.301293
H	3.543856	-2.921901	6.301293
H	0.439789	4.571981	6.301293
H	-3.543856	2.921901	6.301293
H	-5.486221	-3.563102	8.889578
H	-4.108256	-1.701696	9.950306
H	-6.398837	-1.359850	8.889578
H	-5.567801	-3.729851	7.113149
H	-4.041456	-4.027455	7.973429
H	-2.697108	-2.075892	8.916551
H	-3.375021	-0.439266	8.916551
H	-5.705582	-0.009900	7.973429
H	-6.574433	-1.299627	7.113149
H	5.486221	3.563102	8.889578
H	4.108256	1.701696	9.950306

H	6.398837	1.359850	8.889578
H	5.567801	3.729851	7.113149
H	4.041456	4.027455	7.973429
H	2.697108	2.075892	8.916551
H	3.375021	0.439266	8.916551
H	5.705582	0.009900	7.973429
H	6.574433	1.299627	7.113149
H	3.563102	-5.486221	8.889578
H	1.701696	-4.108256	9.950306
H	1.359850	-6.398837	8.889578
H	3.729851	-5.567801	7.113149
H	4.027455	-4.041456	7.973429
H	2.075892	-2.697108	8.916551
H	0.439266	-3.375021	8.916551
H	0.009900	-5.705582	7.973429
H	1.299627	-6.574433	7.113149
H	-3.563102	5.486221	8.889578
H	-1.701696	4.108256	9.950306
H	-1.359850	6.398837	8.889578
H	-3.729851	5.567801	7.113149
H	-4.027455	4.041456	7.973429
H	-2.075892	2.697108	8.916551
H	-0.439266	3.375021	8.916551
H	-0.009900	5.705582	7.973429
H	-1.299627	6.574433	7.113149

Table 3: Cartesian coordinates of **(1)** in C_{4v} broken symmetry GGA Becke Perdew / TZP-ZORA, spin singlet. N.a denotes an α spin-polarised nitrogen atom. N.b denotes a β spin-polarised nitrogen atom. Equilibrium N−N distance 1.263 Å

Atom	X	Y	Z
C	-2.995459	1.264553	-0.064648
C	-1.865670	1.865670	-0.677192
C	-1.264553	2.995459	-0.064648
C	-1.827400	3.518152	1.104608
C	-2.963277	2.963277	1.716721
C	-3.518152	1.827400	1.104608
O	-1.404837	1.404837	-1.852897
Nb	0.000000	0.000000	-2.299647
O	1.404837	1.404837	-1.852897
C	1.865670	1.865670	-0.677192
C	2.995459	1.264553	-0.064648
C	3.518152	1.827400	1.104608
C	2.963277	2.963277	1.716721
C	1.827400	3.518152	1.104608
C	1.264553	2.995459	-0.064648
C	3.599434	0.000000	-0.654533
C	2.995459	-1.264553	-0.064648
C	1.865670	-1.865670	-0.677192
C	1.264553	-2.995459	-0.064648
C	1.827400	-3.518152	1.104608
C	2.963277	-2.963277	1.716721
C	3.518152	-1.827400	1.104608
C	3.505339	3.505339	3.053450
C	5.023599	3.262800	3.192852
C	0.000000	3.599434	-0.654533
O	1.404837	-1.404837	-1.852897
C	0.000000	-3.599434	-0.654533
C	-1.264553	-2.995459	-0.064648
C	-1.865670	-1.865670	-0.677192
C	-2.995459	-1.264553	-0.064648
C	-3.518152	-1.827400	1.104608
C	-2.963277	-2.963277	1.716721
C	-1.827400	-3.518152	1.104608
O	-1.404837	-1.404837	-1.852897
C	-3.599434	0.000000	-0.654533
C	-3.505339	-3.505339	3.053450
C	-5.023599	-3.262800	3.192852
C	3.505339	-3.505339	3.053450
C	3.262800	-5.023599	3.192852
C	-3.505339	3.505339	3.053450
C	-3.262800	5.023599	3.192852
N.a	0.000000	0.000000	-4.125415
Xx	-0.707141	-0.707090	-4.061058
N.b	0.000000	0.000000	-5.387918
Xx	-1.000031	0.000008	-5.451063
Nb	0.000000	0.000000	-7.213687
O	0.000000	1.986783	-7.660378
C	0.000000	2.638617	-8.836058
C	-1.223969	3.012678	-9.448399
C	-1.195591	3.781528	-10.616847
C	0.000000	4.193281	-11.228340
C	1.195591	3.781528	-10.616847
C	1.223969	3.012678	-9.448399
C	-2.544948	2.544948	-8.858267
C	-3.012678	1.223969	-9.448399
C	-2.638617	0.000000	-8.836058
C	-3.012678	-1.223969	-9.448399
C	-3.781528	-1.195591	-10.616847

C	-4.193281	0.000000	-11.228340
C	-3.781528	1.195591	-10.616847
O	-1.986783	0.000000	-7.660378
C	-2.544948	-2.544948	-8.858267
C	-1.223969	-3.012678	-9.448399
C	0.000000	-2.638617	-8.836058
C	1.223969	-3.012678	-9.448399
C	1.195591	-3.781528	-10.616847
C	0.000000	-4.193281	-11.228340
C	-1.195591	-3.781528	-10.616847
C	-4.961486	0.000000	-12.564193
C	-5.863974	-1.244934	-12.702601
O	0.000000	-1.986783	-7.660378
C	2.544948	-2.544948	-8.858267
C	3.012678	-1.223969	-9.448399
C	2.638617	0.000000	-8.836058
C	3.012678	1.223969	-9.448399
C	3.781528	1.195591	-10.616847
C	4.193281	0.000000	-11.228340
C	3.781528	-1.195591	-10.616847
O	1.986783	0.000000	-7.660378
C	2.544948	2.544948	-8.858267
C	4.961486	0.000000	-12.564193
C	5.863974	1.244934	-12.702601
C	0.000000	-4.961486	-12.564193
C	1.244934	-5.863974	-12.702601
C	0.000000	4.961486	-12.564193
C	-1.244934	5.863974	-12.702601
C	5.863974	-1.244934	-12.702601
C	3.940283	0.000000	-13.728004
C	-5.863974	1.244934	-12.702601
C	-3.940283	0.000000	-13.728004
C	-1.244934	-5.863974	-12.702601
C	0.000000	-3.940283	-13.728004
C	1.244934	5.863974	-12.702601
C	0.000000	3.940283	-13.728004
C	-3.262800	-5.023599	3.192852
C	-2.782473	-2.782473	4.216281
C	3.262800	5.023599	3.192852
C	2.782473	2.782473	4.216281
C	5.023599	-3.262800	3.192852
C	2.782473	-2.782473	4.216281
C	-5.023599	3.262800	3.192852
C	-2.782473	2.782473	4.216281
H	3.311139	-3.311139	-9.048189
H	2.430754	-2.430754	-7.774226
H	-3.311139	3.311139	-9.048189
H	-2.430754	2.430754	-7.774226
H	-3.311139	-3.311139	-9.048189
H	-2.430754	-2.430754	-7.774226
H	3.311139	3.311139	-9.048189
H	2.430754	2.430754	-7.774226
H	4.056882	2.155929	-11.057535
H	4.056882	-2.155929	-11.057535
H	-4.056882	-2.155929	-11.057535
H	-4.056882	2.155929	-11.057535
H	2.155929	-4.056882	-11.057535
H	-2.155929	-4.056882	-11.057535
H	-2.155929	4.056882	-11.057535
H	2.155929	4.056882	-11.057535
H	6.437365	-1.192400	-13.642459
H	4.453440	0.000000	-14.705967
H	6.437365	1.192400	-13.642459
H	6.574390	-1.314824	-11.865876
H	5.279433	-2.174392	-12.727515
H	3.291475	-0.885717	-13.673865
H	3.291475	0.885717	-13.673865
H	5.279433	2.174392	-12.727515
H	6.574390	1.314824	-11.865876
H	-6.437365	1.192400	-13.642459
H	-4.453440	0.000000	-14.705967
H	-6.437365	-1.192400	-13.642459
H	-6.574390	1.314824	-11.865876
H	-5.279433	2.174392	-12.727515
H	-3.291475	0.885717	-13.673865
H	-3.291475	-0.885717	-13.673865
H	-5.279433	-2.174392	-12.727515
H	-6.574390	-1.314824	-11.865876
H	-1.192400	-6.437365	-13.642459
H	0.000000	-4.453440	-14.705967
H	1.192400	-6.437365	-13.642459
H	-1.314824	-6.574390	-11.865876
H	-2.174392	-5.279433	-12.727515
H	-0.885717	-3.291475	-13.673865
H	0.885717	-3.291475	-13.673865
H	2.174392	-5.279433	-12.727515
H	1.314824	-6.574390	-11.865876
H	1.192400	6.437365	-13.642459

H	0.000000	4.453440	-14.705967
H	-1.192400	6.437365	-13.642459
H	1.314824	6.574390	-11.865876
H	2.174392	5.279433	-12.727515
H	0.885717	3.291475	-13.673865
H	-0.885717	3.291475	-13.673865
H	-2.174392	5.279433	-12.727515
H	-1.314824	6.574390	-11.865876
H	0.000000	-4.682706	-0.462907
H	0.000000	-3.439939	-1.738922
H	0.000000	4.682706	-0.462907
H	0.000000	3.439939	-1.738922
H	4.682706	0.000000	-0.462907
H	3.439939	0.000000	-1.738922
H	-4.682706	0.000000	-0.462907
H	-3.439939	0.000000	-1.738922
H	-4.391596	-1.342702	1.545542
H	-1.342702	-4.391596	1.545542
H	4.391596	1.342702	1.545542
H	1.342702	4.391596	1.545542
H	1.342702	-4.391596	1.545542
H	4.391596	-1.342702	1.545542
H	-1.342702	4.391596	1.545542
H	-4.391596	1.342702	1.545542
H	-3.704988	-5.391372	4.133094
H	-3.144813	-3.144813	5.194648
H	-5.391372	-3.704988	4.133094
H	-3.715831	-5.576006	2.356640
H	-2.192172	-5.266893	3.217647
H	-1.697440	-2.950049	4.161619
H	-2.950049	-1.697440	4.161619
H	-5.266893	-2.192172	3.217647
H	-5.576006	-3.715831	2.356640
H	3.704988	5.391372	4.133094
H	3.144813	3.144813	5.194648
H	5.391372	3.704988	4.133094
H	3.715831	5.576006	2.356640
H	2.192172	5.266893	3.217647
H	1.697440	2.950049	4.161619
H	2.950049	1.697440	4.161619
H	5.266893	2.192172	3.217647
H	5.576006	3.715831	2.356640
H	5.391372	-3.704988	4.133094
H	3.144813	-3.144813	5.194648
H	3.704988	-5.391372	4.133094
H	5.576006	-3.715831	2.356640
H	5.266893	-2.192172	3.217647
H	2.950049	-1.697440	4.161619
H	1.697440	-2.950049	4.161619
H	2.192172	-5.266893	3.217647
H	3.715831	-5.576006	2.356640
H	-5.391372	3.704988	4.133094
H	-3.144813	3.144813	5.194648
H	-3.704988	5.391372	4.133094
H	-5.576006	3.715831	2.356640
H	-5.266893	2.192172	3.217647
H	-2.950049	1.697440	4.161619
H	-1.697440	2.950049	4.161619
H	-2.192172	5.266893	3.217647
H	-3.715831	5.576006	2.356640

2.3 ADF software geometry optimisations, complex (2), D_{4h} symmetry

Table 4: Cartesian coordinates of **(2)** in D_{4h} Symmetry GGA Becke Perdew / TZ2P-ZORA, spin singlet. Equilibrium N−N distance 1.265 Å

Atom	X	Y	Z
C	-3.039136	1.232413	-4.659014
C	-2.649649	0.000000	-4.066896
C	-3.039136	-1.232413	-4.659014
C	-3.873617	-1.205569	-5.780326
C	-4.308491	0.000000	-6.338020
C	-3.873617	1.205569	-5.780326
O	-1.957094	0.000000	-2.922250
Nb	0.000000	0.000000	-2.450047
O	0.000000	-1.957094	-2.922250
C	0.000000	-2.649649	-4.066896
C	1.232413	-3.039136	-4.659014
C	1.205569	-3.873617	-5.780326
C	0.000000	-4.308491	-6.338020
C	-1.205569	-3.873617	-5.780326
C	-1.232413	-3.039136	-4.659014
C	2.548989	-2.548989	-4.073582
C	3.039136	-1.232413	-4.659014
C	2.649649	0.000000	-4.066896
C	3.039136	1.232413	-4.659014
C	3.873617	1.205569	-5.780326
C	4.308491	0.000000	-6.338020
C	3.873617	-1.205569	-5.780326

C	-2.548989	-2.548989	-4.073582
O	1.957094	0.000000	-2.922250
C	2.548989	2.548989	-4.073582
C	1.232413	3.039136	-4.659014
C	0.000000	2.649649	-4.066896
C	-1.232413	3.039136	-4.659014
C	-1.205569	3.873617	-5.780326
C	0.000000	4.308491	-6.338020
C	1.205569	3.873617	-5.780326
O	0.000000	1.957094	-2.922250
C	-2.548989	2.548989	-4.073582
N	0.000000	0.000000	-0.632250
H	4.970928	0.000000	-7.203959
N	0.000000	0.000000	0.632250
H	-4.970928	0.000000	-7.203959
Nb	0.000000	0.000000	2.450047
O	-1.957094	0.000000	2.922250
C	-2.649649	0.000000	4.066896
C	-3.039136	1.232413	4.659014
C	-3.873617	1.205569	5.780326
C	-4.308491	0.000000	6.338020
C	-3.873617	-1.205569	5.780326
C	-3.039136	-1.232413	4.659014
C	-2.548989	2.548989	4.073582
C	-1.232413	3.039136	4.659014
C	0.000000	2.649649	4.066896
C	1.232413	3.039136	4.659014
C	1.205569	3.873617	5.780326
C	0.000000	4.308491	6.338020
C	-1.205569	3.873617	5.780326
O	0.000000	1.957094	2.922250
C	2.548989	2.548989	4.073582
C	3.039136	1.232413	4.659014
C	2.649649	0.000000	4.066896
C	3.039136	-1.232413	4.659014
C	3.873617	-1.205569	5.780326
C	4.308491	0.000000	6.338020
C	3.873617	1.205569	5.780326
O	1.957094	0.000000	2.922250
C	2.548989	-2.548989	4.073582
C	1.232413	-3.039136	4.659014
C	0.000000	-2.649649	4.066896
C	-1.232413	-3.039136	4.659014
C	-1.205569	-3.873617	5.780326
C	0.000000	-4.308491	6.338020
C	1.205569	-3.873617	5.780326
O	0.000000	-1.957094	2.922250
C	-2.548989	-2.548989	4.073582
H	3.316013	-3.316013	4.253192
H	2.430817	-2.430817	2.990637
H	-3.316013	3.316013	4.253192
H	-2.430817	2.430817	2.990637
H	3.316013	3.316013	4.253192
H	2.430817	2.430817	2.990637
H	-3.316013	-3.316013	4.253192
H	-2.430817	-2.430817	2.990637
H	-2.152613	-4.189227	6.224124
H	2.152613	-4.189227	6.224124
H	0.000000	-4.970928	7.203959
H	2.152613	4.189227	6.224124
H	-2.152613	4.189227	6.224124
H	0.000000	4.970928	7.203959
H	4.189227	-2.152613	6.224124
H	4.189227	2.152613	6.224124
H	4.970928	0.000000	7.203959
H	-4.189227	2.152613	6.224124
H	-4.189227	-2.152613	6.224124
H	-4.970928	0.000000	7.203959
H	3.316013	3.316013	-4.253192
H	2.430817	2.430817	-2.990637
H	-3.316013	-3.316013	-4.253192
H	-2.430817	-2.430817	-2.990637
H	3.316013	-3.316013	-4.253192
H	2.430817	-2.430817	-2.990637
H	-3.316013	3.316013	-4.253192
H	-2.430817	2.430817	-2.990637
H	-2.152613	4.189227	-6.224124
H	2.152613	4.189227	-6.224124
H	2.152613	-4.189227	-6.224124
H	-2.152613	-4.189227	-6.224124
H	4.189227	2.152613	-6.224124
H	4.189227	-2.152613	-6.224124
H	-4.189227	-2.152613	-6.224124
H	-4.189227	2.152613	-6.224124
H	0.000000	4.970928	-7.203959
H	0.000000	-4.970928	-7.203959

Table 5: Cartesian coordinates of **(2)** in D_{4h} Symmetry Hybrid B3LYP / TZP-ZORA, spin singlet. Equilibrium N−N distance 1.263 Å

Atom	X	Y	Z
C	1.261554	-2.990596	-4.705773

C	1.862353	-1.862353	-4.102701
C	2.990596	-1.261554	-4.705773
C	3.518108	-1.824012	-5.863245
C	2.951667	-2.951667	-6.445404
C	1.824012	-3.518108	-5.863245
O	1.396711	-1.396711	-2.939429
Nb	0.000000	0.000000	-2.450611
O	1.396711	1.396711	-2.939429
C	1.862353	1.862353	-4.102701
C	1.261554	2.990596	-4.705773
C	1.824012	3.518108	-5.863245
C	2.951667	2.951667	-6.445404
C	3.518108	1.824012	-5.863245
C	2.990596	1.261554	-4.705773
C	0.000000	3.588527	-4.114275
C	-1.261554	2.990596	-4.705773
C	-1.862353	1.862353	-4.102701
C	-2.990596	1.261554	-4.705773
C	-3.518108	1.824012	-5.863245
C	-2.951667	2.951667	-6.445404
C	-1.824012	3.518108	-5.863245
C	3.588527	0.000000	-4.114275
O	-1.396711	1.396711	-2.939429
C	-3.588527	0.000000	-4.114275
C	-2.990596	-1.261554	-4.705773
C	-1.862353	-1.862353	-4.102701
C	-1.261554	-2.990596	-4.705773
C	-1.824012	-3.518108	-5.863245
C	-2.951667	-2.951667	-6.445404
C	-3.518108	-1.824012	-5.863245
O	-1.396711	-1.396711	-2.939429
C	0.000000	-3.588527	-4.114275
N	0.000000	0.000000	-0.631660
N	0.000000	0.000000	0.631660
Nb	0.000000	0.000000	2.450611
O	1.396711	-1.396711	2.939429
C	1.862353	-1.862353	4.102701
C	1.261554	-2.990596	4.705773
C	1.824012	-3.518108	5.863245
C	2.951667	-2.951667	6.445404
C	3.518108	-1.824012	5.863245
C	2.990596	-1.261554	4.705773
C	0.000000	-3.588527	4.114275
C	-1.261554	-2.990596	4.705773

C	-1.862353	-1.862353	4.102701
C	-2.990596	-1.261554	4.705773
C	-3.518108	-1.824012	5.863245
C	-2.951667	-2.951667	6.445404
C	-1.824012	-3.518108	5.863245
O	-1.396711	-1.396711	2.939429
C	-3.588527	0.000000	4.114275
C	-2.990596	1.261554	4.705773
C	-1.862353	1.862353	4.102701
C	-1.261554	2.990596	4.705773
C	-1.824012	3.518108	5.863245
C	-2.951667	2.951667	6.445404
C	-3.518108	1.824012	5.863245
O	-1.396711	1.396711	2.939429
C	0.000000	3.588527	4.114275
C	1.261554	2.990596	4.705773
C	1.862353	1.862353	4.102701
C	2.990596	1.261554	4.705773
C	3.518108	1.824012	5.863245
C	2.951667	2.951667	6.445404
C	1.824012	3.518108	5.863245
O	1.396711	1.396711	2.939429
C	3.588527	0.000000	4.114275
H	0.000000	4.664774	4.293775
H	0.000000	3.426132	3.039979
H	0.000000	-4.664774	4.293775
H	0.000000	-3.426132	3.039979
H	-4.664774	0.000000	4.293775
H	-3.426132	0.000000	3.039979
H	4.664774	0.000000	4.293775
H	3.426132	0.000000	3.039979
H	4.388773	1.366608	6.318233
H	1.366608	4.388773	6.318233
H	3.377343	3.377343	7.344928
H	-4.388773	-1.366608	6.318233
H	-1.366608	-4.388773	6.318233
H	-3.377343	-3.377343	7.344928
H	-1.366608	4.388773	6.318233
H	-4.388773	1.366608	6.318233
H	-3.377343	3.377343	7.344928
H	1.366608	-4.388773	6.318233
H	4.388773	-1.366608	6.318233
H	3.377343	-3.377343	7.344928
H	-4.664774	0.000000	-4.293775

H	-3.426132	0.000000	-3.039979
H	4.664774	0.000000	-4.293775
H	3.426132	0.000000	-3.039979
H	0.000000	4.664774	-4.293775
H	0.000000	3.426132	-3.039979
H	0.000000	-4.664774	-4.293775
H	0.000000	-3.426132	-3.039979
H	-1.366608	-4.388773	-6.318233
H	-4.388773	-1.366608	-6.318233
H	1.366608	4.388773	-6.318233
H	4.388773	1.366608	-6.318233
H	-4.388773	1.366608	-6.318233
H	-1.366608	4.388773	-6.318233
H	4.388773	-1.366608	-6.318233
H	1.366608	-4.388773	-6.318233
H	-3.377343	-3.377343	-7.344928
H	3.377343	3.377343	-7.344928
H	-3.377343	3.377343	-7.344928
H	3.377343	-3.377343	-7.344928

Table 6: Cartesian coordinates of **(2)** in D_{4h} Symmetry Hybrid B3LYP / TZ2P-ZORA, spin singlet. Equilibrium N−N distance 1.270 Å

Atom	X	Y	Z
C	1.264990	-2.993098	-4.706979
C	1.859985	-1.859985	-4.108629
C	2.993098	-1.264990	-4.706979
C	3.530939	-1.839222	-5.851729
C	2.971417	-2.971417	-6.427491
C	1.839222	-3.530939	-5.851729
O	1.378171	-1.378171	-2.966077
Nb	0.000000	0.000000	-2.444695
O	1.378171	1.378171	-2.966077
C	1.859985	1.859985	-4.108629
C	1.264990	2.993098	-4.706979
C	1.839222	3.530939	-5.851729
C	2.971417	2.971417	-6.427491
C	3.530939	1.839222	-5.851729
C	2.993098	1.264990	-4.706979
C	0.000000	3.589545	-4.121181
C	-1.264990	2.993098	-4.706979
C	-1.859985	1.859985	-4.108629
C	-2.993098	1.264990	-4.706979
C	-3.530939	1.839222	-5.851729
C	-2.971417	2.971417	-6.427491
C	-1.839222	3.530939	-5.851729
C	3.589545	0.000000	-4.121181
O	-1.378171	1.378171	-2.966077
C	-3.589545	0.000000	-4.121181
C	-2.993098	-1.264990	-4.706979
C	-1.859985	-1.859985	-4.108629
C	-1.264990	-2.993098	-4.706979
C	-1.839222	-3.530939	-5.851729
C	-2.971417	-2.971417	-6.427491
C	-3.530939	-1.839222	-5.851729
O	-1.378171	-1.378171	-2.966077
C	0.000000	-3.589545	-4.121181
N	0.000000	0.000000	-0.635115
N	0.000000	0.000000	0.635115
Nb	0.000000	0.000000	2.444695
O	1.378171	-1.378171	2.966077
C	1.859985	-1.859985	4.108629
C	1.264990	-2.993098	4.706979
C	1.839222	-3.530939	5.851729
C	2.971417	-2.971417	6.427491
C	3.530939	-1.839222	5.851729
C	2.993098	-1.264990	4.706979
C	0.000000	-3.589545	4.121181
C	-1.264990	-2.993098	4.706979
C	-1.859985	-1.859985	4.108629
C	-2.993098	-1.264990	4.706979
C	-3.530939	-1.839222	5.851729
C	-2.971417	-2.971417	6.427491
C	-1.839222	-3.530939	5.851729
O	-1.378171	-1.378171	2.966077
C	-3.589545	0.000000	4.121181
C	-2.993098	1.264990	4.706979
C	-1.859985	1.859985	4.108629
C	-1.264990	2.993098	4.706979
C	-1.839222	3.530939	5.851729
C	-2.971417	2.971417	6.427491
C	-3.530939	1.839222	5.851729
O	-1.378171	1.378171	2.966077
C	0.000000	3.589545	4.121181
C	1.264990	2.993098	4.706979
C	1.859985	1.859985	4.108629
C	2.993098	1.264990	4.706979
C	3.530939	1.839222	5.851729
C	2.971417	2.971417	6.427491
C	1.839222	3.530939	5.851729

O	1.378171	1.378171	2.966077
C	3.589545	0.000000	4.121181
H	0.000000	4.664253	4.307224
H	0.000000	3.437097	3.045167
H	0.000000	-4.664253	4.307224
H	0.000000	-3.437097	3.045167
H	-4.664253	0.000000	4.307224
H	-3.437097	0.000000	3.045167
H	4.664253	0.000000	4.307224
H	3.437097	0.000000	3.045167
H	4.405038	1.386899	6.302827
H	1.386899	4.405038	6.302827
H	3.406518	3.406518	7.316517
H	-4.405038	-1.386899	6.302827
H	-1.386899	-4.405038	6.302827
H	-3.406518	-3.406518	7.316517
H	-1.386899	4.405038	6.302827
H	-4.405038	1.386899	6.302827
H	-3.406518	3.406518	7.316517
H	1.386899	-4.405038	6.302827
H	4.405038	-1.386899	6.302827
H	3.406518	-3.406518	7.316517
H	-4.664253	0.000000	-4.307224
H	-3.437097	0.000000	-3.045167
H	4.664253	0.000000	-4.307224
H	3.437097	0.000000	-3.045167
H	0.000000	4.664253	-4.307224
H	0.000000	3.437097	-3.045167
H	0.000000	-4.664253	-4.307224
H	0.000000	-3.437097	-3.045167
H	-1.386899	-4.405038	-6.302827
H	-4.405038	-1.386899	-6.302827
H	1.386899	4.405038	-6.302827
H	4.405038	1.386899	-6.302827
H	-4.405038	1.386899	-6.302827
H	-1.386899	4.405038	-6.302827
H	4.405038	-1.386899	-6.302827
H	1.386899	-4.405038	-6.302827
H	-3.406518	-3.406518	-7.316517
H	3.406518	3.406518	-7.316517
H	-3.406518	3.406518	-7.316517
H	3.406518	-3.406518	-7.316517
C	-2.646806	0.000000	-4.118877
C	-3.039653	-1.232370	-4.708448
C	-3.880903	-1.205537	-5.824681
C	-4.317257	0.000000	-6.381139
C	-3.880903	1.205537	-5.824681
O	-1.951928	0.000000	-2.975993
Nb	0.000000	0.000000	-2.492449
O	0.000000	-1.951928	-2.975993
C	0.000000	-2.646806	-4.118877
C	1.232370	-3.039653	-4.708448
C	1.205537	-3.880903	-5.824681
C	0.000000	-4.317257	-6.381139
C	-1.205537	-3.880903	-5.824681
C	-1.232370	-3.039653	-4.708448
C	2.549575	-2.549575	-4.124136
C	3.039653	-1.232370	-4.708448
C	2.646806	0.000000	-4.118877
C	3.039653	1.232370	-4.708448
C	3.880903	1.205537	-5.824681
C	4.317257	0.000000	-6.381139
C	3.880903	-1.205537	-5.824681
C	-2.549575	-2.549575	-4.124136
O	1.951928	0.000000	-2.975993
C	2.549575	2.549575	-4.124136
C	1.232370	3.039653	-4.708448
C	0.000000	2.646806	-4.118877
C	-1.232370	3.039653	-4.708448
C	-1.205537	3.880903	-5.824681
C	0.000000	4.317257	-6.381139
C	1.205537	3.880903	-5.824681
O	0.000000	1.951928	-2.975993
C	-2.549575	2.549575	-4.124136
N	0.000000	0.000000	-0.695000
H	4.983007	0.000000	-7.244311
N	0.000000	0.000000	0.695000
H	-4.983007	0.000000	-7.244311
Nb	0.000000	0.000000	2.492449
O	-1.951928	0.000000	2.975993
C	-2.646806	0.000000	4.118877
C	-3.039653	1.232370	4.708448
C	-3.880903	1.205537	5.824681
C	-4.317257	0.000000	6.381139
C	-3.880903	-1.205537	5.824681
C	-3.039653	-1.232370	4.708448

Table 7: Cartesian coordinates of **(2)** in D_{4h} Symmetry GGA Becke Perdew / TZ2P-ZORA, spin singlet, with N−N distance constrained to 1.39 Å

Atom	X	Y	Z
C	-3.039653	1.232370	-4.708448

C	-2.549575	2.549575	4.124136
C	-1.232370	3.039653	4.708448
C	0.000000	2.646806	4.118877
C	1.232370	3.039653	4.708448
C	1.205537	3.880903	5.824681
C	0.000000	4.317257	6.381139
C	-1.205537	3.880903	5.824681
O	0.000000	1.951928	2.975993
C	2.549575	2.549575	4.124136
C	3.039653	1.232370	4.708448
C	2.646806	0.000000	4.118877
C	3.039653	-1.232370	4.708448
C	3.880903	-1.205537	5.824681
C	4.317257	0.000000	6.381139
C	3.880903	1.205537	5.824681
O	1.951928	0.000000	2.975993
C	2.549575	-2.549575	4.124136
C	1.232370	-3.039653	4.708448
C	0.000000	-2.646806	4.118877
C	-1.232370	-3.039653	4.708448
C	-1.205537	-3.880903	5.824681
C	0.000000	-4.317257	6.381139
C	1.205537	-3.880903	5.824681
O	0.000000	-1.951928	2.975993
C	-2.549575	-2.549575	4.124136
H	3.316159	-3.316159	4.306014
H	2.433144	-2.433144	3.040475
H	-3.316159	3.316159	4.306014
H	-2.433144	2.433144	3.040475
H	3.316159	3.316159	4.306014
H	2.433144	2.433144	3.040475
H	-3.316159	-3.316159	4.306014
H	-2.433144	-2.433144	3.040475
H	-2.152821	-4.201167	6.264856
H	2.152821	-4.201167	6.264856
H	0.000000	-4.983007	7.244311
H	2.152821	4.201167	6.264856
H	-2.152821	4.201167	6.264856
H	0.000000	4.983007	7.244311
H	4.201167	-2.152821	6.264856
H	4.201167	2.152821	6.264856
H	4.983007	0.000000	7.244311
H	-4.201167	2.152821	6.264856
H	-4.201167	-2.152821	6.264856
H	-4.983007	0.000000	7.244311
H	3.316159	3.316159	-4.306014
H	2.433144	2.433144	-3.040475
H	-3.316159	-3.316159	-4.306014
H	-2.433144	-2.433144	-3.040475
H	3.316159	-3.316159	-4.306014
H	2.433144	-2.433144	-3.040475
H	-3.316159	3.316159	-4.306014
H	-2.433144	2.433144	-3.040475
H	-2.152821	4.201167	-6.264856
H	2.152821	4.201167	-6.264856
H	2.152821	-4.201167	-6.264856
H	-2.152821	-4.201167	-6.264856
H	4.201167	2.152821	-6.264856
H	4.201167	-2.152821	-6.264856
H	-4.201167	-2.152821	-6.264856
H	-4.201167	2.152821	-6.264856
H	0.000000	4.983007	-7.244311
H	0.000000	-4.983007	-7.244311

2.4 ADF software geometry optimisations, complex (2), D_{4d} symmetry

Table 8: Cartesian coordinates of **(2)** in D_{4d} Symmetry GGA Becke Perdew / TZ2P-ZORA, spin singlet, equilibrium N−N distance is 1.266 Å

Atom	X	Y	Z
C	-2.332226	-2.299376	4.671972
C	-2.444926	-1.012722	4.077314
C	-3.275037	-0.023229	4.671972
C	-4.027947	-0.363958	5.799780
C	-3.961524	-1.640917	6.363805
C	-3.105546	-2.590831	5.799780
O	-1.808681	-0.749180	2.929486
Nb	0.000000	0.000000	2.452925
O	-0.749180	1.808681	2.929486
C	-1.012722	2.444926	4.077314
C	-0.023229	3.275037	4.671972
C	-0.363958	4.027947	5.799780
C	-1.640917	3.961524	6.363805
C	-2.590831	3.105546	5.799780
C	-2.299376	2.332226	4.671972
C	1.379265	3.329839	4.085398
C	2.332226	2.299376	4.671972
C	2.444926	1.012722	4.077314
C	3.275037	0.023229	4.671972

C	4.027947	0.363958	5.799780
C	3.961524	1.640917	6.363805
C	3.105546	2.590831	5.799780
C	-3.329839	1.379265	4.085398
O	1.808681	0.749180	2.929486
C	3.329839	-1.379265	4.085398
C	2.299376	-2.332226	4.671972
C	1.012722	-2.444926	4.077314
C	0.023229	-3.275037	4.671972
C	0.363958	-4.027947	5.799780
C	1.640917	-3.961524	6.363805
C	2.590831	-3.105546	5.799780
O	0.749180	-1.808681	2.929486
C	-1.379265	-3.329839	4.085398
N	0.000000	0.000000	0.632975
H	4.562728	1.889944	7.238529
N	0.000000	0.000000	-0.632975
H	-4.562728	-1.889944	7.238529
Nb	0.000000	0.000000	-2.452925
O	-1.808681	0.749180	-2.929486
C	-2.444926	1.012722	-4.077314
C	-3.275037	0.023229	-4.671972
C	-4.027947	0.363958	-5.799780
C	-3.961524	1.640917	-6.363805
C	-3.105546	2.590831	-5.799780
C	-2.332226	2.299376	-4.671972
C	-3.329839	-1.379265	-4.085398
C	-2.299376	-2.332226	-4.671972
C	-1.012722	-2.444926	-4.077314
C	-0.023229	-3.275037	-4.671972
C	-0.363958	-4.027947	-5.799780
C	-1.640917	-3.961524	-6.363805
C	-2.590831	-3.105546	-5.799780
O	-0.749180	-1.808681	-2.929486
C	1.379265	-3.329839	-4.085398
C	2.332226	-2.299376	-4.671972
C	2.444926	-1.012722	-4.077314
C	3.275037	-0.023229	-4.671972
C	4.027947	-0.363958	-5.799780
C	3.961524	-1.640917	-6.363805
C	3.105546	-2.590831	-5.799780
O	1.808681	-0.749180	-2.929486
C	3.329839	1.379265	-4.085398
C	2.299376	2.332226	-4.671972
C	1.012722	2.444926	-4.077314
C	0.023229	3.275037	-4.671972
C	0.363958	4.027947	-5.799780
C	1.640917	3.961524	-6.363805
C	2.590831	3.105546	-5.799780
O	0.749180	1.808681	-2.929486
C	-1.379265	3.329839	-4.085398
H	4.331724	1.794259	-4.266824
H	3.176190	1.315621	-3.001947
H	-4.331724	-1.794259	-4.266824
H	-3.176190	-1.315621	-3.001947
H	1.794259	-4.331724	-4.266824
H	1.315621	-3.176190	-3.001947
H	-1.794259	4.331724	-4.266824
H	-1.315621	3.176190	-3.001947
H	-0.391372	4.680235	-6.244396
H	3.586168	3.032684	-6.244396
H	1.889944	4.562728	-7.238529
H	0.391372	-4.680235	-6.244396
H	-3.586168	-3.032684	-6.244396
H	-1.889944	-4.562728	-7.238529
H	4.680235	0.391372	-6.244396
H	3.032684	-3.586168	-6.244396
H	4.562728	-1.889944	-7.238529
H	-4.680235	-0.391372	-6.244396
H	-3.032684	3.586168	-6.244396
H	-4.562728	1.889944	-7.238529
H	4.331724	-1.794259	4.266824
H	3.176190	-1.315621	3.001947
H	-4.331724	1.794259	4.266824
H	-3.176190	1.315621	3.001947
H	1.794259	4.331724	4.266824
H	1.315621	3.176190	3.001947
H	-1.794259	-4.331724	4.266824
H	-1.315621	-3.176190	3.001947
H	-0.391372	-4.680235	6.244396
H	3.586168	-3.032684	6.244396
H	0.391372	4.680235	6.244396
H	-3.586168	3.032684	6.244396
H	4.680235	-0.391372	6.244396
H	3.032684	3.586168	6.244396
H	-4.680235	0.391372	6.244396
H	-3.032684	-3.586168	6.244396
H	1.889944	-4.562728	7.238529

H	-1.889944	4.562728	7.238529

2.5 Asymmetric mono– and disubstituted geometries

Table 9: Cartesian coordinates of dianionic **(2)**H_2 C_s Symmetry GGA Becke Perdew / TZP-ZORA, spin singlet, equilibrium N−N distance equals 1.441 Å

Atom	X	Y	Z
C	0.150836	0.005664	3.880915
C	1.269452	0.076638	3.042630
C	1.736046	1.360720	2.651375
C	1.048135	2.542518	3.037824
C	-0.066584	2.415876	3.876043
C	-0.512653	1.162005	4.309650
C	1.999731	-1.175169	2.563642
C	1.498895	-1.724323	1.231602
C	2.096443	-1.319742	0.000000
C	1.498895	-1.724323	-1.231602
C	0.434862	-2.634895	-1.204279
C	-0.087302	-3.116644	0.000000
C	0.434862	-2.634895	1.204279
C	1.999731	-1.175169	-2.563642
C	1.269452	0.076638	-3.042630
C	1.736046	1.360720	-2.651375
C	1.048135	2.542518	-3.037824
C	-0.066584	2.415876	-3.876043
C	-0.512653	1.162005	-4.309650
C	0.150836	0.005664	-3.880915
C	1.545313	3.905206	-2.561380
C	0.957945	4.379702	-1.235135
C	1.592384	4.050541	0.000000
C	0.957945	4.379702	1.235135
C	-0.208226	5.152514	1.206782
C	-0.784020	5.566988	0.000000
C	-0.208226	5.152514	-1.206782
O	2.802171	3.475103	0.000000
Nb.a	3.322546	1.497184	0.000000
O	2.881592	1.460342	-1.960304
C	1.545313	3.905206	2.561380
O	3.225551	-0.587344	0.000000
O	2.881592	1.460342	1.960304
N	5.285439	1.432620	0.000000
N	6.155966	0.284747	0.000000
Nb.b	8.119163	0.238816	0.000000
O	8.563482	0.279484	-1.956356
C	9.702182	0.391528	-2.656628
C	10.395960	-0.784582	-3.048514
C	11.508971	-0.648615	-3.887078
C	11.946803	0.610052	-4.316370
C	11.274405	1.760685	-3.886212
C	10.155855	1.679527	-3.048272
C	9.912022	-2.147690	-2.562707
C	10.512840	-2.597765	-1.234245
C	11.714502	-3.314224	-1.206008
C	12.311855	-3.697346	0.000000
C	11.714502	-3.314224	1.206008
C	10.512840	-2.597765	1.234245
C	9.864757	-2.291730	0.000000
O	8.635433	-1.752442	0.000000
C	9.912022	-2.147690	2.562707
C	10.395960	-0.784582	3.048514
C	9.702182	0.391528	2.656628
C	10.155855	1.679527	3.048272
C	11.274405	1.760685	3.886212
C	11.946803	0.610052	4.316370
C	11.508971	-0.648615	3.887078
C	9.417090	2.923566	-2.564434
C	9.917709	3.468875	-1.231166
C	9.320962	3.062999	0.000000
C	9.917709	3.468875	1.231166
C	10.985518	4.374813	1.204105
C	11.510440	4.853582	0.000000
C	10.985518	4.374813	-1.204105
O	8.194482	2.325711	0.000000
C	9.417090	2.923566	2.564434
O	8.563482	0.279484	1.956356
Xx	6.419211	0.839261	0.986847
Xx	5.025045	0.917978	0.987302
H	5.893538	2.260182	0.000000
H	5.549987	-0.544084	0.000000
H	10.162975	-2.896519	-3.329108
H	8.820496	-2.114504	-2.462412
H	9.530758	3.709949	3.325915
H	8.350282	2.686923	2.473501
H	9.530758	3.709949	-3.325915
H	8.350282	2.686923	-2.473501
H	10.162975	-2.896519	3.329108

H	8.820496	-2.114504	2.462412
H	12.193832	-3.574508	2.154260
H	12.193832	-3.574508	-2.154260
H	13.240585	-4.270760	0.000000
H	11.416611	4.708160	-2.152666
H	11.416611	4.708160	2.152666
H	12.331278	5.573434	0.000000
H	12.040933	-1.547185	-4.212121
H	11.623152	2.744882	-4.211412
H	12.810519	0.694452	-4.978797
H	11.623152	2.744882	4.211412
H	12.040933	-1.547185	4.212121
H	12.810519	0.694452	4.978797
H	1.299089	4.649538	-3.333686
H	2.637215	3.861486	-2.466836
H	1.880219	-1.957359	3.328549
H	3.068175	-0.945498	2.473026
H	1.880219	-1.957359	-3.328549
H	3.068175	-0.945498	-2.473026
H	1.299089	4.649538	3.333686
H	2.637215	3.861486	2.466836
H	-0.672629	5.438741	2.154988
H	-0.672629	5.438741	-2.154988
H	0.005475	-2.971714	-2.152431
H	0.005475	-2.971714	2.152431
H	-0.590260	3.319060	-4.201153
H	-0.204123	-0.974969	-4.209083
H	-0.204123	-0.974969	4.209083
H	-0.590260	3.319060	4.201153
H	-1.679561	6.190281	0.000000
H	-0.903304	-3.841775	0.000000
H	-1.374170	1.085598	-4.975721
H	-1.374170	1.085598	4.975721

Table 10: Cartesian coordinates of neutral **(2)**H_2 C_s Symmetry GGA Becke Perdew / TZP-ZORA, spin singlet, equilibrium N−N distance equals 1.396 Å

Atom	X	Y	Z
C	0.057053	-0.044684	3.833782
C	1.191894	0.007757	3.015572
C	1.679426	1.279933	2.632041
C	1.019254	2.471637	3.015609
C	-0.112529	2.365914	3.832503
C	-0.589670	1.121370	4.250205
C	1.889441	-1.266502	2.554792
C	1.358657	-1.817828	1.239035
C	1.878007	-1.377688	0.000000
C	1.358657	-1.817828	-1.239035
C	0.331721	-2.769048	-1.210394
C	-0.172198	-3.251292	0.000000
C	0.331721	-2.769048	1.210394
C	1.889441	-1.266502	-2.554792
C	1.191894	0.007757	-3.015572
C	1.679426	1.279933	-2.632041
C	1.019254	2.471637	-3.015609
C	-0.112529	2.365914	-3.832503
C	-0.589670	1.121370	-4.250205
C	0.057053	-0.044684	-3.833782
C	1.534300	3.830546	-2.556083
C	0.934492	4.306187	-1.239906
C	1.509124	3.941537	0.000000
C	0.934492	4.306187	1.239906
C	-0.211489	5.109731	1.210897
C	-0.775926	5.519605	0.000000
C	-0.211489	5.109731	-1.210897
O	2.679144	3.237250	0.000000
Nb.a	3.283642	1.398777	0.000000
O	2.841399	1.363030	-1.928152
C	1.534300	3.830546	2.556083
O	2.939462	-0.515472	0.000000
O	2.841399	1.363030	1.928152
N	5.270566	1.503581	0.000000
N	6.165139	0.431397	0.000000
Nb.b	8.153486	0.473792	0.000000
O	8.602215	0.478344	-1.927646
C	9.768683	0.485983	-2.629078
C	10.353809	-0.745006	-3.010777
C	11.494970	-0.711019	-3.820875
C	12.053486	0.500763	-4.234886
C	11.477836	1.705100	-3.823506
C	10.337141	1.724006	-3.012023
C	9.751566	-2.068775	-2.555974
C	10.316244	-2.582581	-1.239107
C	11.406677	-3.459891	-1.210282
C	11.942728	-3.906562	0.000000
C	11.406677	-3.459891	1.210282
C	10.316244	-2.582581	1.239107
C	9.765817	-2.180187	0.000000
O	8.644652	-1.399366	0.000000
C	9.751566	-2.068775	2.555974
C	10.353809	-0.745006	3.010777

C	9.768683	0.485983	2.629078
C	10.337141	1.724006	3.012023
C	11.477836	1.705100	3.823506
C	12.053486	0.500763	4.234886
C	11.494970	-0.711019	3.820875
C	9.717003	3.039393	-2.556718
C	10.275296	3.556593	-1.238658
C	9.724491	3.154120	0.000000
C	10.275296	3.556593	1.238658
C	11.366534	4.433359	1.209889
C	11.902920	4.879923	0.000000
C	11.366534	4.433359	-1.209889
O	8.606650	2.365368	0.000000
C	9.717003	3.039393	2.556718
O	8.602215	0.478344	1.927646
Xx	6.419938	0.838398	0.986798
Xx	5.025787	0.917779	0.986842
H	5.775199	2.394759	0.000000
H	5.655709	-0.457639	0.000000
H	9.945345	-2.822785	-3.330343
H	8.664918	-1.954086	-2.467055
H	9.902450	3.796452	3.330126
H	8.631858	2.910440	2.469553
H	9.902450	3.796452	-3.330126
H	8.631858	2.910440	-2.469553
H	9.945345	-2.822785	3.330343
H	8.664918	-1.954086	2.467055
H	11.837494	-3.801737	2.152910
H	11.837494	-3.801737	-2.152910
H	12.783937	-4.599346	0.000000
H	11.798672	4.772863	-2.152783
H	11.798672	4.772863	2.152783
H	12.745850	5.570468	0.000000
H	11.947722	-1.652240	-4.138989
H	11.916719	2.651834	-4.144517
H	12.934231	0.506211	-4.876512
H	11.916719	2.651834	4.144517
H	11.947722	-1.652240	4.138989
H	12.934231	0.506211	4.876512
H	1.296108	4.571610	-3.330508
H	2.625822	3.784934	-2.463537
H	1.756946	-2.034226	3.328577
H	2.964036	-1.070037	2.461304
H	1.756946	-2.034226	-3.328577
H	2.964036	-1.070037	-2.461304
H	1.296108	4.571610	3.330508
H	2.625822	3.784934	2.463537
H	-0.663535	5.423050	2.153544
H	-0.663535	5.423050	-2.153544
H	-0.072551	-3.142128	-2.153067
H	-0.072551	-3.142128	2.153067
H	-0.622436	3.276468	-4.153396
H	-0.320951	-1.017223	-4.155415
H	-0.320951	-1.017223	4.155415
H	-0.622436	3.276468	4.153396
H	-1.661094	6.155530	0.000000
H	-0.960514	-4.004143	0.000000
H	-1.464238	1.060561	-4.897481
H	-1.464238	1.060561	4.897481

Table 11: Cartesian coordinates of anionic **(2)**H C_s Symmetry GGA Becke Perdew / TZP-ZORA, spin singlet, equilibrium N−N distance equals 1.327 Å

Atom	X	Y	Z
C	5.856386	3.916937	1.211319
C	4.744168	3.067265	1.239859
C	4.195177	2.668863	0.000000
C	4.744168	3.067265	-1.239859
C	5.856386	3.916937	-1.211319
C	6.408431	4.344314	0.000000
C	4.136491	2.581392	2.548767
C	4.684057	1.244892	3.032897
C	4.063404	0.025997	2.652594
C	4.621907	-1.219952	3.039951
C	5.750959	-1.219668	3.867554
C	6.339676	-0.026489	4.294438
C	5.810276	1.192343	3.862618
C	4.011705	-2.528283	2.555298
C	4.593974	-3.017912	1.236893
C	4.036378	-2.613513	0.000000
C	4.593974	-3.017912	-1.236893
C	5.706262	-3.869176	-1.208722
C	6.259259	-4.298811	0.000000
C	5.706262	-3.869176	1.208722
C	4.011705	-2.528283	-2.555298
C	4.621907	-1.219952	-3.039951
C	4.063404	0.025997	-2.652594
C	4.684057	1.244892	-3.032897
C	5.810276	1.192343	-3.862618

C	6.339676	-0.026489	-4.294438
C	5.750959	-1.219668	-3.867554
O	2.896828	0.055667	-1.966269
Nb	2.469995	0.061277	0.000000
O	3.070571	1.908243	0.000000
C	4.136491	2.581392	-2.548767
O	2.911614	-1.838233	0.000000
O	2.896828	0.055667	1.966269
N	0.536059	0.479693	0.000000
N	-0.624165	-0.164139	0.000000
Nb	-2.467836	-0.104284	0.000000
O	-2.935740	-2.040492	0.000000
C	-4.122473	-2.692484	0.000000
C	-4.713934	-3.059690	1.235975
C	-5.856276	-3.868885	1.208233
C	-6.420900	-4.287638	0.000000
C	-5.856276	-3.868885	-1.208233
C	-4.713934	-3.059690	-1.235975
C	-4.121027	-2.581070	2.555791
C	-4.684569	-1.250762	3.040055
C	-4.068069	-0.031201	2.653654
C	-4.632307	1.215458	3.034746
C	-5.763835	1.214177	3.859574
C	-6.349786	0.020726	4.290153
C	-5.812945	-1.198993	3.866213
C	-4.025019	2.524824	2.550001
C	-4.607592	3.022112	1.234175
C	-4.045592	2.609215	0.000000
C	-4.607592	3.022112	-1.234175
C	-5.714344	3.880189	-1.207751
C	-6.267051	4.315976	0.000000
C	-5.714344	3.880189	1.207751
O	-2.928785	1.842470	0.000000
C	-4.025019	2.524824	-2.550001
C	-4.632307	1.215458	-3.034746
C	-4.068069	-0.031201	-2.653654
C	-4.684569	-1.250762	-3.040055
C	-5.812945	-1.198993	-3.866213
C	-6.349786	0.020726	-4.290153
C	-5.763835	1.214177	-3.859574
C	-4.121027	-2.581070	-2.555791
O	-2.902329	-0.066097	-1.973534
O	-2.902329	-0.066097	1.973534
XX	0.000000	0.000000	0.000000
H	0.430727	1.509675	0.000000
H	4.332549	3.337726	3.321262
H	3.049621	2.494738	2.432434
H	4.189073	-3.300074	-3.317292
H	2.928058	-2.403059	-2.447950
H	4.189073	-3.300074	3.317292
H	2.928058	-2.403059	2.447950
H	4.332549	3.337726	-3.321262
H	3.049621	2.494738	-2.432434
H	6.292891	4.250444	-2.154945
H	6.292891	4.250444	2.154945
H	7.271636	5.008209	0.000000
H	6.144839	-4.200121	2.152825
H	6.144839	-4.200121	-2.152825
H	7.123712	-4.963424	0.000000
H	6.277585	2.127944	4.178027
H	6.172997	-2.175559	4.186357
H	7.209468	-0.046121	4.951683
H	6.172997	-2.175559	-4.186357
H	6.277585	2.127944	-4.178027
H	7.209468	-0.046121	-4.951683
H	-4.322383	-3.342750	3.322716
H	-3.034118	-2.486140	2.446697
H	-4.196423	3.294097	-3.317075
H	-2.942560	2.393592	-2.435142
H	-4.196423	3.294097	3.317075
H	-2.942560	2.393592	2.435142
H	-4.322383	-3.342750	-3.322716
H	-3.034118	-2.486140	-2.446697
H	-6.308227	-4.177976	-2.153916
H	-6.308227	-4.177976	2.153916
H	-6.149160	4.212252	2.153779
H	-6.149160	4.212252	-2.153779
H	-6.278320	-2.134966	4.184670
H	-6.190800	2.170667	4.171540
H	-6.190800	2.170667	-4.171540
H	-6.278320	-2.134966	-4.184670
H	-7.303454	-4.928370	0.000000
H	-7.126833	4.986997	0.000000
H	-7.222931	0.040916	4.943445
H	-7.222931	0.040916	-4.943445

Table 12: Cartesian coordinates of anionic **(2)**H C_s Symmetry GGA Becke Perdew / TZP-ZORA, spin singlet, equilibrium N−N distance equals 1.327 Å

Atom	X	Y	Z
C	5.797822	3.848178	1.205506

C	4.646428	3.052304	1.232367
C	4.021247	2.700947	0.000000
C	4.646428	3.052304	-1.232367
C	5.797822	3.848178	-1.205506
C	6.368323	4.269564	0.000000
C	4.078456	2.557320	2.556958
C	4.670357	1.235865	3.034325
C	4.074724	0.005975	2.646197
C	4.640114	-1.236604	3.040241
C	5.772329	-1.221099	3.864561
C	6.351814	-0.019018	4.283640
C	5.801394	1.196509	3.858775
C	4.024574	-2.544543	2.558533
C	4.591504	-3.042953	1.234912
C	3.989263	-2.656079	0.000000
C	4.591504	-3.042953	-1.234912
C	5.720395	-3.868179	-1.206946
C	6.284758	-4.299405	0.000000
C	5.720395	-3.868179	1.206946
C	4.024574	-2.544543	-2.558533
C	4.640114	-1.236604	-3.040241
C	4.074724	0.005975	-2.646197
C	4.670357	1.235865	-3.034325
C	5.801394	1.196509	-3.858775
C	6.351814	-0.019018	-4.283640
C	5.772329	-1.221099	-3.864561
O	2.927792	0.018745	-1.944622
Nb	2.463914	0.033749	0.000000
O	2.839307	2.068359	0.000000
C	4.078456	2.557320	-2.556958
O	2.838012	-1.967386	0.000000
O	2.927792	0.018745	1.944622
N	0.549283	0.649820	0.000000
N	-0.632378	0.009540	0.000000
Nb	-2.436679	-0.074586	0.000000
O	-2.881364	-2.049969	0.000000
C	-4.067986	-2.686484	0.000000
C	-4.676639	-3.051918	1.234035
C	-5.830348	-3.845153	1.206371
C	-6.404447	-4.258523	0.000000
C	-5.830348	-3.845153	-1.206371
C	-4.676639	-3.051918	-1.234035
C	-4.088069	-2.578564	2.557227
C	-4.657071	-1.250692	3.040977
C	-4.032930	-0.027969	2.659897
C	-4.619889	1.215098	3.035376
C	-5.759960	1.207379	3.847149
C	-6.346824	0.011214	4.272978
C	-5.796299	-1.204869	3.852393
C	-4.018418	2.526912	2.548830
C	-4.606623	3.022837	1.234408
C	-4.030529	2.618918	0.000000
C	-4.606623	3.022837	-1.234408
C	-5.726967	3.862096	-1.207632
C	-6.287686	4.291692	0.000000
C	-5.726967	3.862096	1.207632
O	-2.900818	1.890693	0.000000
C	-4.018418	2.526912	-2.548830
C	-4.619889	1.215098	-3.035376
C	-4.032930	-0.027969	-2.659897
C	-4.657071	-1.250692	-3.040977
C	-5.796299	-1.204869	-3.852393
C	-6.346824	0.011214	-4.272978
C	-5.759960	1.207379	-3.847149
C	-4.088069	-2.578564	-2.557227
O	-2.864148	-0.050023	-2.004246
O	-2.864148	-0.050023	2.004246
XX	0.000000	0.000000	0.000000
H	0.412718	1.674335	0.000000
H	4.270744	3.320022	3.327102
H	2.992786	2.440553	2.455162
H	4.199529	-3.314058	-3.325252
H	2.941874	-2.409609	-2.452696
H	4.199529	-3.314058	3.325252
H	2.941874	-2.409609	2.452696
H	4.270744	3.320022	-3.327102
H	2.992786	2.440553	-2.455162
H	6.259703	4.138800	-2.153333
H	6.259703	4.138800	2.153333
H	7.258721	4.901019	0.000000
H	6.171603	-4.175499	2.154933
H	6.171603	-4.175499	-2.154933
H	7.162639	-4.948074	0.000000
H	6.260049	2.138104	4.172937
H	6.208020	-2.172614	4.181612
H	7.230983	-0.028396	4.930730
H	6.208020	-2.172614	-4.181612
H	6.260049	2.138104	-4.172937

H	7.230983	-0.028396	-4.930730
H	-4.289870	-3.344578	3.321527
H	-3.001355	-2.479639	2.449069
H	-4.185922	3.296013	-3.317973
H	-2.936937	2.394785	-2.426411
H	-4.185922	3.296013	3.317973
H	-2.936937	2.394785	2.426411
H	-4.289870	-3.344578	-3.321527
H	-3.001355	-2.479639	-2.449069
H	-6.286901	-4.144204	-2.154086
H	-6.286901	-4.144204	2.154086
H	-6.168989	4.183119	2.154999
H	-6.168989	4.183119	-2.154999
H	-6.263317	-2.144597	4.160554
H	-6.197850	2.163168	4.148989
H	-6.197850	2.163168	-4.148989
H	-6.263317	-2.144597	-4.160554
H	-7.297328	-4.886589	0.000000
H	-7.160582	4.947111	0.000000
H	-7.230641	0.026885	4.913339
H	-7.230641	0.026885	-4.913339

2.6 Extra geometries

Table 13: Cartesian coordinates of μ^2−$N_2[Nb(OH)_4]_2$ D_{4h} Symmetry GGA Becke Perdew / TZ2P-ZORA, spin singlet, equilibrium N−N distance equals 1.279 Å

Atom	X	Y	Z
N	0.000000	0.000000	-0.639688
N	0.000000	0.000000	0.639688
Nb	0.000000	0.000000	-2.451152
Nb	0.000000	0.000000	2.451152
O	-1.993511	0.000000	2.964541
O	1.993511	0.000000	2.964541
O	-1.993511	0.000000	-2.964541
O	1.993511	0.000000	-2.964541
O	0.000000	-1.993511	2.964541
O	0.000000	1.993511	2.964541
O	0.000000	-1.993511	-2.964541
O	0.000000	1.993511	-2.964541
H	2.163114	0.000000	3.920591
H	-2.163114	0.000000	3.920591
H	-2.163114	0.000000	-3.920591
H	2.163114	0.000000	-3.920591
H	0.000000	2.163114	-3.920591
H	0.000000	-2.163114	-3.920591
H	0.000000	2.163114	3.920591
H	0.000000	-2.163114	3.920591

Table 14: Cartesian coordinates of μ^2−$N_2[Nb(OCH_3)_4]_2$ D_{4h} Symmetry GGA Becke Perdew / TZ2P-ZORA, spin singlet, equilibrium N−N distance equals 1.280 Å

Atom	X	Y	Z
N	0.000000	0.000000	0.635881
N	0.000000	0.000000	-0.635881
Nb	0.000000	0.000000	2.454523
Nb	0.000000	0.000000	-2.454523
O	0.000000	1.988968	2.949974
O	0.000000	-1.988968	2.949974
O	0.000000	1.988968	-2.949974
O	0.000000	-1.988968	-2.949974
O	-1.988968	0.000000	-2.949974
O	1.988968	0.000000	-2.949974
O	-1.988968	0.000000	2.949974
O	1.988968	0.000000	2.949974
H	0.000000	1.792352	5.051505
H	0.000000	-1.792352	5.051505
H	0.000000	1.792352	-5.051505
H	0.000000	-1.792352	-5.051505
H	-3.180377	0.894147	-4.392058
H	3.180377	0.894147	-4.392058
H	-1.792352	0.000000	5.051505
H	1.792352	0.000000	5.051505
C	2.537015	0.000000	4.216048
H	3.180377	-0.894147	4.392058
H	3.180377	0.894147	4.392058
C	-2.537015	0.000000	4.216048
H	-3.180377	0.894147	4.392058
H	-3.180377	-0.894147	4.392058
C	2.537015	0.000000	-4.216048
H	3.180377	-0.894147	-4.392058
H	1.792352	0.000000	-5.051505
C	-2.537015	0.000000	-4.216048
H	-1.792352	0.000000	-5.051505
H	-3.180377	-0.894147	-4.392058
C	0.000000	-2.537015	-4.216048
H	0.894147	-3.180377	-4.392058
H	-0.894147	-3.180377	-4.392058

C	0.000000	2.537015	-4.216048
H	-0.894147	3.180377	-4.392058
H	0.894147	3.180377	-4.392058
C	0.000000	-2.537015	4.216048
H	-0.894147	-3.180377	4.392058
H	0.894147	-3.180377	4.392058
C	0.000000	2.537015	4.216048
H	0.894147	3.180377	4.392058
H	-0.894147	3.180377	4.392058

2.7 GAUSSIAN auxiliary geometries

Table 15: Cartesian coordinates of **(2)** D_{4d} Symmetry B3LYP / SDDAll, spin singlet, equilibrium N−N distance equals 1.283 Å

Atom	X	Y	Z
N	0.000000	0.000000	0.641339
Nb	0.000000	0.000000	2.456983
O	0.000000	1.949699	3.025147
O	-1.949699	0.000000	3.025147
O	0.000000	-1.949699	3.025147
O	1.949699	0.000000	3.025147
C	0.000000	2.665261	4.185181
C	1.233184	3.043839	4.777523
C	1.208195	3.850427	5.923806
C	0.000000	4.264426	6.496377
C	-1.208195	3.850427	5.923806
C	-1.233184	3.043839	4.777523
C	0.000000	-2.665261	4.185181
C	-1.233184	-3.043839	4.777523
C	-1.208195	-3.850427	5.923806
C	0.000000	-4.264426	6.496377
C	1.208195	-3.850427	5.923806
C	1.233184	-3.043839	4.777523
C	-2.665261	0.000000	4.185181
C	-3.043839	1.233184	4.777523
C	-3.850427	1.208195	5.923806
C	-4.264426	0.000000	6.496377
C	-3.850427	-1.208195	5.923806
C	-3.043839	-1.233184	4.777523
C	2.665261	0.000000	4.185181
C	3.043839	-1.233184	4.777523
C	3.850427	-1.208195	5.923806
C	4.264426	0.000000	6.496377
C	3.850427	1.208195	5.923806
C	3.043839	1.233184	4.777523
C	-2.557642	2.557642	4.191210
C	-2.557642	-2.557642	4.191210
C	2.557642	-2.557642	4.191210
C	2.557642	2.557642	4.191210
H	-3.321296	3.321296	4.384663
H	-2.449979	2.449979	3.108752
H	3.321296	-3.321296	4.384663
H	2.449979	-2.449979	3.108752
H	-3.321296	-3.321296	4.384663
H	-2.449979	-2.449979	3.108752
H	3.321296	3.321296	4.384663
H	2.449979	2.449979	3.108752
H	2.151586	4.152738	6.373502
H	-2.151586	4.152738	6.373502
H	0.000000	4.894872	7.381438
H	-2.151586	-4.152738	6.373502
H	2.151586	-4.152738	6.373502
H	0.000000	-4.894872	7.381438
H	-4.152738	2.151586	6.373502
H	-4.152738	-2.151586	6.373502
H	-4.894872	0.000000	7.381438
H	4.152738	-2.151586	6.373502
H	4.152738	2.151586	6.373502
H	4.894872	0.000000	7.381438
N	0.000000	0.000000	-0.641339
Nb	0.000000	0.000000	-2.456983
O	1.378646	1.378646	-3.025147
O	1.378646	-1.378646	-3.025147
O	-1.378646	-1.378646	-3.025147
O	-1.378646	1.378646	-3.025147
C	1.884624	1.884624	-4.185181
C	1.280327	3.024312	-4.777523
C	1.868341	3.576986	-5.923806
C	3.015404	3.015404	-6.496377
C	3.576986	1.868341	-5.923806
C	3.024312	1.280327	-4.777523
C	-1.884624	-1.884624	-4.185181
C	-1.280327	-3.024312	-4.777523
C	-1.868341	-3.576986	-5.923806
C	-3.015404	-3.015404	-6.496377
C	-3.576986	-1.868341	-5.923806
C	-3.024312	-1.280327	-4.777523
C	1.884624	-1.884624	-4.185181

C	3.024312	-1.280327	-4.777523
C	3.576986	-1.868341	-5.923806
C	3.015404	-3.015404	-6.496377
C	1.868341	-3.576986	-5.923806
C	1.280327	-3.024312	-4.777523
C	-1.884624	1.884624	-4.185181
C	-3.024312	1.280327	-4.777523
C	-3.576986	1.868341	-5.923806
C	-3.015404	3.015404	-6.496377
C	-1.868341	3.576986	-5.923806
C	-1.280327	3.024312	-4.777523
C	3.617053	0.000000	-4.191210
C	0.000000	-3.617053	-4.191210
C	-3.617053	0.000000	-4.191210
C	0.000000	3.617053	-4.191210
H	4.697022	0.000000	-4.384663
H	3.464793	0.000000	-3.108752
H	-4.697022	0.000000	-4.384663
H	-3.464793	0.000000	-3.108752
H	0.000000	-4.697022	-4.384663
H	0.000000	-3.464793	-3.108752
H	0.000000	4.697022	-4.384663
H	0.000000	3.464793	-3.108752
H	1.415028	4.457830	-6.373502
H	4.457830	1.415028	-6.373502
H	-1.415028	-4.457830	-6.373502
H	-4.457830	-1.415028	-6.373502
H	4.457830	-1.415028	-6.373502
H	1.415028	-4.457830	-6.373502
H	-4.457830	1.415028	-6.373502
H	-1.415028	4.457830	-6.373502
H	3.461197	3.461197	-7.381438
H	-3.461197	-3.461197	-7.381438
H	3.461197	-3.461197	-7.381438
H	-3.461197	3.461197	-7.381438

Table 16: Cartesian coordinates of **(2)** D_{4h} Symmetry ωB97XD / SDDAll, spin singlet, equilibrium N−N distance equals 1.292 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.428272
Nb	0.000000	0.000000	-2.428272
N	0.000000	0.000000	-0.645906
N	0.000000	0.000000	0.645906
C	1.227167	3.017564	-4.741998
C	0.000000	2.647333	-4.146569
C	-1.227167	3.017564	-4.741998
C	-1.204951	3.787575	-5.908529
C	0.000000	4.182093	-6.493882
C	1.204951	3.787575	-5.908529
O	-1.943127	0.000000	-2.988907
O	0.000000	1.943127	-2.988907
C	-2.647333	0.000000	-4.146569
C	-3.017564	-1.227167	-4.741998
C	-3.787575	-1.204951	-5.908529
C	-4.182093	0.000000	-6.493882
C	-3.787575	1.204951	-5.908529
C	-3.017564	1.227167	-4.741998
C	-2.542371	-2.542371	-4.144918
C	-1.227167	-3.017564	-4.741998
C	0.000000	-2.647333	-4.146569
C	1.227167	-3.017564	-4.741998
C	1.204951	-3.787575	-5.908529
C	0.000000	-4.182093	-6.493882
C	-1.204951	-3.787575	-5.908529
C	-2.542371	2.542371	-4.144918
O	0.000000	-1.943127	-2.988907
C	2.542371	-2.542371	-4.144918
C	3.017564	-1.227167	-4.741998
C	2.647333	0.000000	-4.146569
C	3.017564	1.227167	-4.741998
C	3.787575	1.204951	-5.908529
C	4.182093	0.000000	-6.493882
C	3.787575	-1.204951	-5.908529
O	1.943127	0.000000	-2.988907
C	2.542371	2.542371	-4.144918
H	0.000000	-4.781623	-7.400325
H	0.000000	4.781623	-7.400325
O	0.000000	1.943127	2.988907
C	0.000000	2.647333	4.146569
C	1.227167	3.017564	4.741998
C	1.204951	3.787575	5.908529
C	0.000000	4.182093	6.493882
C	-1.204951	3.787575	5.908529
C	-1.227167	3.017564	4.741998
C	2.542371	2.542371	4.144918
C	3.017564	1.227167	4.741998
C	2.647333	0.000000	4.146569
C	3.017564	-1.227167	4.741998
C	3.787575	-1.204951	5.908529
C	4.182093	0.000000	6.493882

C	3.787575	1.204951	5.908529
O	1.943127	0.000000	2.988907
C	2.542371	-2.542371	4.144918
C	1.227167	-3.017564	4.741998
C	0.000000	-2.647333	4.146569
C	-1.227167	-3.017564	4.741998
C	-1.204951	-3.787575	5.908529
C	0.000000	-4.182093	6.493882
C	1.204951	-3.787575	5.908529
O	0.000000	-1.943127	2.988907
C	-2.542371	-2.542371	4.144918
C	-3.017564	-1.227167	4.741998
C	-2.647333	0.000000	4.146569
C	-3.017564	1.227167	4.741998
C	-3.787575	1.204951	5.908529
C	-4.182093	0.000000	6.493882
C	-3.787575	-1.204951	5.908529
O	-1.943127	0.000000	2.988907
C	-2.542371	2.542371	4.144918
H	-3.307727	-3.307727	4.324449
H	-2.424261	-2.424261	3.063956
H	3.307727	3.307727	4.324449
H	2.424261	2.424261	3.063956
H	3.307727	-3.307727	4.324449
H	2.424261	-2.424261	3.063956
H	-3.307727	3.307727	4.324449
H	-2.424261	2.424261	3.063956
H	-4.073082	2.150202	6.365968
H	-4.073082	-2.150202	6.365968
H	-4.781623	0.000000	7.400325
H	4.073082	-2.150202	6.365968
H	4.073082	2.150202	6.365968
H	4.781623	0.000000	7.400325
H	-2.150202	-4.073082	6.365968
H	2.150202	-4.073082	6.365968
H	0.000000	-4.781623	7.400325
H	2.150202	4.073082	6.365968
H	-2.150202	4.073082	6.365968
H	0.000000	4.781623	7.400325
H	3.307727	-3.307727	-4.324449
H	2.424261	-2.424261	-3.063956
H	-3.307727	3.307727	-4.324449
H	-2.424261	2.424261	-3.063956
H	-3.307727	-3.307727	-4.324449
H	-2.424261	-2.424261	-3.063956
H	3.307727	3.307727	-4.324449
H	2.424261	2.424261	-3.063956
H	4.073082	2.150202	-6.365968
H	4.073082	-2.150202	-6.365968
H	-4.073082	-2.150202	-6.365968
H	-4.073082	2.150202	-6.365968
H	2.150202	-4.073082	-6.365968
H	-2.150202	-4.073082	-6.365968
H	-2.150202	4.073082	-6.365968
H	2.150202	4.073082	-6.365968
H	4.781623	0.000000	-7.400325
H	-4.781623	0.000000	-7.400325

Table 17: Cartesian coordinates of **(2)** D_{4h} Symmetry LC-ωPBE / SDDAll, spin singlet, equilibrium N−N distance equals 1.301 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.418956
Nb	0.000000	0.000000	-2.418956
N	0.000000	0.000000	-0.650527
N	0.000000	0.000000	0.650527
C	1.222769	3.009405	-4.738900
C	0.000000	2.636904	-4.149742
C	-1.222769	3.009405	-4.738900
C	-1.200987	3.795617	-5.888608
C	0.000000	4.199050	-6.464334
C	1.200987	3.795617	-5.888608
O	-1.923676	0.000000	-3.002503
O	0.000000	1.923676	-3.002503
C	-2.636904	0.000000	-4.149742
C	-3.009405	-1.222769	-4.738900
C	-3.795617	-1.200987	-5.888608
C	-4.199050	0.000000	-6.464334
C	-3.795617	1.200987	-5.888608
C	-3.009405	1.222769	-4.738900
C	-2.530294	-2.530294	-4.142488
C	-1.222769	-3.009405	-4.738900
C	0.000000	-2.636904	-4.149742
C	1.222769	-3.009405	-4.738900
C	1.200987	-3.795617	-5.888608
C	0.000000	-4.199050	-6.464334
C	-1.200987	-3.795617	-5.888608
C	-2.530294	2.530294	-4.142488
O	0.000000	-1.923676	-3.002503

C	2.530294	-2.530294	-4.142488
C	3.009405	-1.222769	-4.738900
C	2.636904	0.000000	-4.149742
C	3.009405	1.222769	-4.738900
C	3.795617	1.200987	-5.888608
C	4.199050	0.000000	-6.464334
C	3.795617	-1.200987	-5.888608
O	1.923676	0.000000	-3.002503
C	2.530294	2.530294	-4.142488
H	0.000000	-4.814563	-7.358550
H	0.000000	4.814563	-7.358550
O	0.000000	1.923676	3.002503
C	0.000000	2.636904	4.149742
C	1.222769	3.009405	4.738900
C	1.200987	3.795617	5.888608
C	0.000000	4.199050	6.464334
C	-1.200987	3.795617	5.888608
C	-1.222769	3.009405	4.738900
C	2.530294	2.530294	4.142488
C	3.009405	1.222769	4.738900
C	2.636904	0.000000	4.149742
C	3.009405	-1.222769	4.738900
C	3.795617	-1.200987	5.888608
C	4.199050	0.000000	6.464334
C	3.795617	1.200987	5.888608
O	1.923676	0.000000	3.002503
C	2.530294	-2.530294	4.142488
C	1.222769	-3.009405	4.738900
C	0.000000	-2.636904	4.149742
C	-1.222769	-3.009405	4.738900
C	-1.200987	-3.795617	5.888608
C	0.000000	-4.199050	6.464334
C	1.200987	-3.795617	5.888608
O	0.000000	-1.923676	3.002503
C	-2.530294	-2.530294	4.142488
C	-3.009405	-1.222769	4.738900
C	-2.636904	0.000000	4.149742
C	-3.009405	1.222769	4.738900
C	-3.795617	1.200987	5.888608
C	-4.199050	0.000000	6.464334
C	-3.795617	-1.200987	5.888608
O	-1.923676	0.000000	3.002503
C	-2.530294	2.530294	4.142488
H	-3.295406	-3.295406	4.309737
H	-2.403238	-2.403238	3.064830
H	3.295406	3.295406	4.309737
H	2.403238	2.403238	3.064830
H	3.295406	-3.295406	4.309737
H	2.403238	-2.403238	3.064830
H	-3.295406	3.295406	4.309737
H	-2.403238	2.403238	3.064830
H	-4.090666	2.145154	6.339723
H	-4.090666	-2.145154	6.339723
H	-4.814563	0.000000	7.358550
H	4.090666	-2.145154	6.339723
H	4.090666	2.145154	6.339723
H	4.814563	0.000000	7.358550
H	-2.145154	-4.090666	6.339723
H	2.145154	-4.090666	6.339723
H	0.000000	-4.814563	7.358550
H	2.145154	4.090666	6.339723
H	-2.145154	4.090666	6.339723
H	0.000000	4.814563	7.358550
H	3.295406	-3.295406	-4.309737
H	2.403238	-2.403238	-3.064830
H	-3.295406	3.295406	-4.309737
H	-2.403238	2.403238	-3.064830
H	-3.295406	-3.295406	-4.309737
H	-2.403238	-2.403238	-3.064830
H	3.295406	3.295406	-4.309737
H	2.403238	2.403238	-3.064830
H	4.090666	2.145154	-6.339723
H	4.090666	-2.145154	-6.339723
H	-4.090666	-2.145154	-6.339723
H	-4.090666	2.145154	-6.339723
H	2.145154	-4.090666	-6.339723
H	-2.145154	-4.090666	-6.339723
H	-2.145154	4.090666	-6.339723
H	2.145154	4.090666	-6.339723
H	4.814563	0.000000	-7.358550
H	-4.814563	0.000000	-7.358550

Table 18: Cartesian coordinates of **(2)** D_{4h} Symmetry CAM-B3LYP / SDDAll, spin singlet, equilibrium N−N distance equals 1.296 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.438687
Nb	0.000000	0.000000	-2.438687
N	0.000000	0.000000	-0.647911
N	0.000000	0.000000	0.647911
C	1.227523	3.028916	-4.761753

C	0.000000	2.651961	-4.173109
C	-1.227523	3.028916	-4.761753
C	-1.204447	3.827912	-5.907760
C	0.000000	4.237803	-6.481154
C	1.204447	3.827912	-5.907760
O	-1.932204	0.000000	-3.021172
O	0.000000	1.932204	-3.021172
C	-2.651961	0.000000	-4.173109
C	-3.028916	-1.227523	-4.761753
C	-3.827912	-1.204447	-5.907760
C	-4.237803	0.000000	-6.481154
C	-3.827912	1.204447	-5.907760
C	-3.028916	1.227523	-4.761753
C	-2.544461	-2.544461	-4.171382
C	-1.227523	-3.028916	-4.761753
C	0.000000	-2.651961	-4.173109
C	1.227523	-3.028916	-4.761753
C	1.204447	-3.827912	-5.907760
C	0.000000	-4.237803	-6.481154
C	-1.204447	-3.827912	-5.907760
C	-2.544461	2.544461	-4.171382
O	0.000000	-1.932204	-3.021172
C	2.544461	-2.544461	-4.171382
C	3.028916	-1.227523	-4.761753
C	2.651961	0.000000	-4.173109
C	3.028916	1.227523	-4.761753
C	3.827912	1.204447	-5.907760
C	4.237803	0.000000	-6.481154
C	3.827912	-1.204447	-5.907760
O	1.932204	0.000000	-3.021172
C	2.544461	2.544461	-4.171382
H	0.000000	-4.862685	-7.369531
H	0.000000	4.862685	-7.369531
O	0.000000	1.932204	3.021172
C	0.000000	2.651961	4.173109
C	1.227523	3.028916	4.761753
C	1.204447	3.827912	5.907760
C	0.000000	4.237803	6.481154
C	-1.204447	3.827912	5.907760
C	-1.227523	3.028916	4.761753
C	2.544461	2.544461	4.171382
C	3.028916	1.227523	4.761753
C	2.651961	0.000000	4.173109
C	3.028916	-1.227523	4.761753
C	3.827912	-1.204447	5.907760
C	4.237803	0.000000	6.481154
C	3.827912	1.204447	5.907760
O	1.932204	0.000000	3.021172
C	2.544461	-2.544461	4.171382
C	1.227523	-3.028916	4.761753
C	0.000000	-2.651961	4.173109
C	-1.227523	-3.028916	4.761753
C	-1.204447	-3.827912	5.907760
C	0.000000	-4.237803	6.481154
C	1.204447	-3.827912	5.907760
O	0.000000	-1.932204	3.021172
C	-2.544461	-2.544461	4.171382
C	-3.028916	-1.227523	4.761753
C	-2.651961	0.000000	4.173109
C	-3.028916	1.227523	4.761753
C	-3.827912	1.204447	5.907760
C	-4.237803	0.000000	6.481154
C	-3.827912	-1.204447	5.907760
O	-1.932204	0.000000	3.021172
C	-2.544461	2.544461	4.171382
H	-3.308901	-3.308901	4.354258
H	-2.427876	-2.427876	3.091131
H	3.308901	3.308901	4.354258
H	2.427876	2.427876	3.091131
H	3.308901	-3.308901	4.354258
H	2.427876	-2.427876	3.091131
H	-3.308901	3.308901	4.354258
H	-2.427876	2.427876	3.091131
H	-4.127205	2.148688	6.356857
H	-4.127205	-2.148688	6.356857
H	-4.862685	0.000000	7.369531
H	4.127205	-2.148688	6.356857
H	4.127205	2.148688	6.356857
H	4.862685	0.000000	7.369531
H	-2.148688	-4.127205	6.356857
H	2.148688	-4.127205	6.356857
H	0.000000	-4.862685	7.369531
H	2.148688	4.127205	6.356857
H	-2.148688	4.127205	6.356857
H	0.000000	4.862685	7.369531
H	3.308901	-3.308901	-4.354258
H	2.427876	-2.427876	-3.091131
H	-3.308901	3.308901	-4.354258

H	-2.427876	2.427876	-3.091131
H	-3.308901	-3.308901	-4.354258
H	-2.427876	-2.427876	-3.091131
H	3.308901	3.308901	-4.354258
H	2.427876	2.427876	-3.091131
H	4.127205	2.148688	-6.356857
H	4.127205	-2.148688	-6.356857
H	-4.127205	-2.148688	-6.356857
H	-4.127205	2.148688	-6.356857
H	2.148688	-4.127205	-6.356857
H	-2.148688	-4.127205	-6.356857
H	-2.148688	4.127205	-6.356857
H	2.148688	4.127205	-6.356857
H	4.862685	0.000000	-7.369531
H	-4.862685	0.000000	-7.369531

Table 19: Cartesian coordinates of **(2)** D_{4h} Symmetry M062X / SDDAll, spin singlet, equilibrium N−N distance equals 1.284 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.418886
Nb	0.000000	0.000000	-2.418886
N	0.000000	0.000000	-0.641917
N	0.000000	0.000000	0.641917
C	1.224971	3.010851	-4.746080
C	0.000000	2.636740	-4.149841
C	-1.224971	3.010851	-4.746080
C	-1.204068	3.784110	-5.909091
C	0.000000	4.180792	-6.492828
C	1.204068	3.784110	-5.909091
O	-1.934264	0.000000	-3.001648
O	0.000000	1.934264	-3.001648
C	-2.636740	0.000000	-4.149841
C	-3.010851	-1.224971	-4.746080
C	-3.784110	-1.204068	-5.909091
C	-4.180792	0.000000	-6.492828
C	-3.784110	1.204068	-5.909091
C	-3.010851	1.224971	-4.746080
C	-2.534935	-2.534935	-4.147953
C	-1.224971	-3.010851	-4.746080
C	0.000000	-2.636740	-4.149841
C	1.224971	-3.010851	-4.746080
C	1.204068	-3.784110	-5.909091
C	0.000000	-4.180792	-6.492828
C	-1.204068	-3.784110	-5.909091
C	-2.534935	2.534935	-4.147953
O	0.000000	-1.934264	-3.001648
C	2.534935	-2.534935	-4.147953
C	3.010851	-1.224971	-4.746080
C	2.636740	0.000000	-4.149841
C	3.010851	1.224971	-4.746080
C	3.784110	1.204068	-5.909091
C	4.180792	0.000000	-6.492828
C	3.784110	-1.204068	-5.909091
O	1.934264	0.000000	-3.001648
C	2.534935	2.534935	-4.147953
H	0.000000	-4.784521	-7.394232
H	0.000000	4.784521	-7.394232
O	0.000000	1.934264	3.001648
C	0.000000	2.636740	4.149841
C	1.224971	3.010851	4.746080
C	1.204068	3.784110	5.909091
C	0.000000	4.180792	6.492828
C	-1.204068	3.784110	5.909091
C	-1.224971	3.010851	4.746080
C	2.534935	2.534935	4.147953
C	3.010851	1.224971	4.746080
C	2.636740	0.000000	4.149841
C	3.010851	-1.224971	4.746080
C	3.784110	-1.204068	5.909091
C	4.180792	0.000000	6.492828
C	3.784110	1.204068	5.909091
O	1.934264	0.000000	3.001648
C	2.534935	-2.534935	4.147953
C	1.224971	-3.010851	4.746080
C	0.000000	-2.636740	4.149841
C	-1.224971	-3.010851	4.746080
C	-1.204068	-3.784110	5.909091
C	0.000000	-4.180792	6.492828
C	1.204068	-3.784110	5.909091
O	0.000000	-1.934264	3.001648
C	-2.534935	-2.534935	4.147953
C	-3.010851	-1.224971	4.746080
C	-2.636740	0.000000	4.149841
C	-3.010851	1.224971	4.746080
C	-3.784110	1.204068	5.909091
C	-4.180792	0.000000	6.492828
C	-3.784110	-1.204068	5.909091
O	-1.934264	0.000000	3.001648

C	-2.534935	2.534935	4.147953
H	-3.299245	-3.299245	4.323248
H	-2.410632	-2.410632	3.069069
H	3.299245	3.299245	4.323248
H	2.410632	2.410632	3.069069
H	3.299245	-3.299245	4.323248
H	2.410632	-2.410632	3.069069
H	-3.299245	3.299245	4.323248
H	-2.410632	2.410632	3.069069
H	-4.072823	2.149706	6.361280
H	-4.072823	-2.149706	6.361280
H	-4.784521	0.000000	7.394232
H	4.072823	-2.149706	6.361280
H	4.072823	2.149706	6.361280
H	4.784521	0.000000	7.394232
H	-2.149706	-4.072823	6.361280
H	2.149706	-4.072823	6.361280
H	0.000000	-4.784521	7.394232
H	2.149706	4.072823	6.361280
H	-2.149706	4.072823	6.361280
H	0.000000	4.784521	7.394232
H	3.299245	-3.299245	-4.323248
H	2.410632	-2.410632	-3.069069
H	-3.299245	3.299245	-4.323248
H	-2.410632	2.410632	-3.069069
H	-3.299245	-3.299245	-4.323248
H	-2.410632	-2.410632	-3.069069
H	3.299245	3.299245	-4.323248
H	2.410632	2.410632	-3.069069
H	4.072823	2.149706	-6.361280
H	4.072823	-2.149706	-6.361280
H	-4.072823	-2.149706	-6.361280
H	-4.072823	2.149706	-6.361280
H	2.149706	-4.072823	-6.361280
H	-2.149706	-4.072823	-6.361280
H	-2.149706	4.072823	-6.361280
H	2.149706	4.072823	-6.361280
H	4.784521	0.000000	-7.394232
H	-4.784521	0.000000	-7.394232

Table 20: Cartesian coordinates of **(2)** D_{4h} Symmetry M06L / SDDAll, spin singlet, equilibrium N−N distance equals 1.276 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.458548
Nb	0.000000	0.000000	-2.458548
N	0.000000	0.000000	-0.637888
N	0.000000	0.000000	0.637888
C	1.230764	3.020576	-4.771078
C	0.000000	2.650154	-4.171464
C	-1.230764	3.020576	-4.771078
C	-1.207519	3.788476	-5.942183
C	0.000000	4.184142	-6.528307
C	1.207519	3.788476	-5.942183
O	-1.964558	0.000000	-3.000636
O	0.000000	1.964558	-3.000636
C	-2.650154	0.000000	-4.171464
C	-3.020576	-1.230764	-4.771078
C	-3.788476	-1.207519	-5.942183
C	-4.184142	0.000000	-6.528307
C	-3.788476	1.207519	-5.942183
C	-3.020576	1.230764	-4.771078
C	-2.544930	-2.544930	-4.174739
C	-1.230764	-3.020576	-4.771078
C	0.000000	-2.650154	-4.171464
C	1.230764	-3.020576	-4.771078
C	1.207519	-3.788476	-5.942183
C	0.000000	-4.184142	-6.528307
C	-1.207519	-3.788476	-5.942183
C	-2.544930	2.544930	-4.174739
O	0.000000	-1.964558	-3.000636
C	2.544930	-2.544930	-4.174739
C	3.020576	-1.230764	-4.771078
C	2.650154	0.000000	-4.171464
C	3.020576	1.230764	-4.771078
C	3.788476	1.207519	-5.942183
C	4.184142	0.000000	-6.528307
C	3.788476	-1.207519	-5.942183
O	1.964558	0.000000	-3.000636
C	2.544930	2.544930	-4.174739
H	0.000000	-4.786310	-7.434421
H	0.000000	4.786310	-7.434421
O	0.000000	1.964558	3.000636
C	0.000000	2.650154	4.171464
C	1.230764	3.020576	4.771078
C	1.207519	3.788476	5.942183
C	0.000000	4.184142	6.528307
C	-1.207519	3.788476	5.942183
C	-1.230764	3.020576	4.771078
C	2.544930	2.544930	4.174739
C	3.020576	1.230764	4.771078

C	2.650154	0.000000	4.171464
C	3.020576	-1.230764	4.771078
C	3.788476	-1.207519	5.942183
C	4.184142	0.000000	6.528307
C	3.788476	1.207519	5.942183
O	1.964558	0.000000	3.000636
C	2.544930	-2.544930	4.174739
C	1.230764	-3.020576	4.771078
C	0.000000	-2.650154	4.171464
C	-1.230764	-3.020576	4.771078
C	-1.207519	-3.788476	5.942183
C	0.000000	-4.184142	6.528307
C	1.207519	-3.788476	5.942183
O	0.000000	-1.964558	3.000636
C	-2.544930	-2.544930	4.174739
C	-3.020576	-1.230764	4.771078
C	-2.650154	0.000000	4.171464
C	-3.020576	1.230764	4.771078
C	-3.788476	1.207519	5.942183
C	-4.184142	0.000000	6.528307
C	-3.788476	-1.207519	5.942183
O	-1.964558	0.000000	3.000636
C	-2.544930	2.544930	4.174739
H	-3.310855	-3.310855	4.357959
H	-2.425407	-2.425407	3.093080
H	3.310855	3.310855	4.357959
H	2.425407	2.425407	3.093080
H	3.310855	-3.310855	4.357959
H	2.425407	-2.425407	3.093080
H	-3.310855	3.310855	4.357959
H	-2.425407	2.425407	3.093080
H	-4.074151	2.155503	6.398950
H	-4.074151	-2.155503	6.398950
H	-4.786310	0.000000	7.434421
H	4.074151	-2.155503	6.398950
H	4.074151	2.155503	6.398950
H	4.786310	0.000000	7.434421
H	-2.155503	-4.074151	6.398950
H	2.155503	-4.074151	6.398950
H	0.000000	-4.786310	7.434421
H	2.155503	4.074151	6.398950
H	-2.155503	4.074151	6.398950
H	0.000000	4.786310	7.434421
H	3.310855	-3.310855	-4.357959
H	2.425407	-2.425407	-3.093080
H	-3.310855	3.310855	-4.357959
H	-2.425407	2.425407	-3.093080
H	-3.310855	-3.310855	-4.357959
H	-2.425407	-2.425407	-3.093080
H	3.310855	3.310855	-4.357959
H	2.425407	2.425407	-3.093080
H	4.074151	2.155503	-6.398950
H	4.074151	-2.155503	-6.398950
H	-4.074151	-2.155503	-6.398950
H	-4.074151	2.155503	-6.398950
H	2.155503	-4.074151	-6.398950
H	-2.155503	-4.074151	-6.398950
H	-2.155503	4.074151	-6.398950
H	2.155503	4.074151	-6.398950
H	4.786310	0.000000	-7.434421
H	-4.786310	0.000000	-7.434421

Table 21: Cartesian coordinates of **(2)** D_{4h} Symmetry M06 / SDDAll, spin singlet, equilibrium N−N distance equals 1.283 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.444288
Nb	0.000000	0.000000	-2.444288
N	0.000000	0.000000	-0.641322
N	0.000000	0.000000	0.641322
C	1.230647	3.019501	-4.752908
C	0.000000	2.643675	-4.154156
C	-1.230647	3.019501	-4.752908
C	-1.207406	3.797909	-5.918353
C	0.000000	4.198852	-6.502670
C	1.207406	3.797909	-5.918353
O	-1.953928	0.000000	-2.990263
O	0.000000	1.953928	-2.990263
C	-2.643675	0.000000	-4.154156
C	-3.019501	-1.230647	-4.752908
C	-3.797909	-1.207406	-5.918353
C	-4.198852	0.000000	-6.502670
C	-3.797909	1.207406	-5.918353
C	-3.019501	1.230647	-4.752908
C	-2.550104	-2.550104	-4.163355
C	-1.230647	-3.019501	-4.752908
C	0.000000	-2.643675	-4.154156
C	1.230647	-3.019501	-4.752908
C	1.207406	-3.797909	-5.918353

C	0.000000	-4.198852	-6.502670
C	-1.207406	-3.797909	-5.918353
C	-2.550104	2.550104	-4.163355
O	0.000000	-1.953928	-2.990263
C	2.550104	-2.550104	-4.163355
C	3.019501	-1.230647	-4.752908
C	2.643675	0.000000	-4.154156
C	3.019501	1.230647	-4.752908
C	3.797909	1.207406	-5.918353
C	4.198852	0.000000	-6.502670
C	3.797909	-1.207406	-5.918353
O	1.953928	0.000000	-2.990263
C	2.550104	2.550104	-4.163355
H	0.000000	-4.809964	-7.405471
H	0.000000	4.809964	-7.405471
O	0.000000	1.953928	2.990263
C	0.000000	2.643675	4.154156
C	1.230647	3.019501	4.752908
C	1.207406	3.797909	5.918353
C	0.000000	4.198852	6.502670
C	-1.207406	3.797909	5.918353
C	-1.230647	3.019501	4.752908
C	2.550104	2.550104	4.163355
C	3.019501	1.230647	4.752908
C	2.643675	0.000000	4.154156
C	3.019501	-1.230647	4.752908
C	3.797909	-1.207406	5.918353
C	4.198852	0.000000	6.502670
C	3.797909	1.207406	5.918353
O	1.953928	0.000000	2.990263
C	2.550104	-2.550104	4.163355
C	1.230647	-3.019501	4.752908
C	0.000000	-2.643675	4.154156
C	-1.230647	-3.019501	4.752908
C	-1.207406	-3.797909	5.918353
C	0.000000	-4.198852	6.502670
C	1.207406	-3.797909	5.918353
O	0.000000	-1.953928	2.990263
C	-2.550104	-2.550104	4.163355
C	-3.019501	-1.230647	4.752908
C	-2.643675	0.000000	4.154156
C	-3.019501	1.230647	4.752908
C	-3.797909	1.207406	5.918353
C	-4.198852	0.000000	6.502670
C	-3.797909	-1.207406	5.918353
O	-1.953928	0.000000	2.990263
C	-2.550104	2.550104	4.163355
H	-3.315288	-3.315288	4.367111
H	-2.446912	-2.446912	3.074908
H	3.315288	3.315288	4.367111
H	2.446912	2.446912	3.074908
H	3.315288	-3.315288	4.367111
H	2.446912	-2.446912	3.074908
H	-3.315288	3.315288	4.367111
H	-2.446912	2.446912	3.074908
H	-4.091057	2.157962	6.370561
H	-4.091057	-2.157962	6.370561
H	-4.809964	0.000000	7.405471
H	4.091057	-2.157962	6.370561
H	4.091057	2.157962	6.370561
H	4.809964	0.000000	7.405471
H	-2.157962	-4.091057	6.370561
H	2.157962	-4.091057	6.370561
H	0.000000	-4.809964	7.405471
H	2.157962	4.091057	6.370561
H	-2.157962	4.091057	6.370561
H	0.000000	4.809964	7.405471
H	3.315288	-3.315288	-4.367111
H	2.446912	-2.446912	-3.074908
H	-3.315288	3.315288	-4.367111
H	-2.446912	2.446912	-3.074908
H	-3.315288	-3.315288	-4.367111
H	-2.446912	-2.446912	-3.074908
H	3.315288	3.315288	-4.367111
H	2.446912	2.446912	-3.074908
H	4.091057	2.157962	-6.370561
H	4.091057	-2.157962	-6.370561
H	-4.091057	-2.157962	-6.370561
H	-4.091057	2.157962	-6.370561
H	2.157962	-4.091057	-6.370561
H	-2.157962	-4.091057	-6.370561
H	-2.157962	4.091057	-6.370561
H	2.157962	4.091057	-6.370561
H	4.809964	0.000000	-7.405471
H	-4.809964	0.000000	-7.405471

Table 22: Cartesian coordinates of **(2)** D_{4h} Symmetry PBE1PBE (PBE0) / SDDAll, spin singlet, equilibrium N−N distance equals 1.277 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.437125

Nb	0.000000	0.000000	-2.437125
N	0.000000	0.000000	-0.638291
N	0.000000	0.000000	0.638291
C	1.227674	3.019626	-4.739987
C	0.000000	2.643663	-4.147958
C	-1.227674	3.019626	-4.739987
C	-1.204241	3.811293	-5.890705
C	0.000000	4.217901	-6.466178
C	1.204241	3.811293	-5.890705
O	-1.938505	0.000000	-2.994670
O	0.000000	1.938505	-2.994670
C	-2.643663	0.000000	-4.147958
C	-3.019626	-1.227674	-4.739987
C	-3.811293	-1.204241	-5.890705
C	-4.217901	0.000000	-6.466178
C	-3.811293	1.204241	-5.890705
C	-3.019626	1.227674	-4.739987
C	-2.538400	-2.538400	-4.147890
C	-1.227674	-3.019626	-4.739987
C	0.000000	-2.643663	-4.147958
C	1.227674	-3.019626	-4.739987
C	1.204241	-3.811293	-5.890705
C	0.000000	-4.217901	-6.466178
C	-1.204241	-3.811293	-5.890705
C	-2.538400	2.538400	-4.147890
O	0.000000	-1.938505	-2.994670
C	2.538400	-2.538400	-4.147890
C	3.019626	-1.227674	-4.739987
C	2.643663	0.000000	-4.147958
C	3.019626	1.227674	-4.739987
C	3.811293	1.204241	-5.890705
C	4.217901	0.000000	-6.466178
C	3.811293	-1.204241	-5.890705
O	1.938505	0.000000	-2.994670
C	2.538400	2.538400	-4.147890
H	0.000000	-4.837543	-7.357702
H	0.000000	4.837543	-7.357702
O	0.000000	1.938505	2.994670
C	0.000000	2.643663	4.147958
C	1.227674	3.019626	4.739987
C	1.204241	3.811293	5.890705
C	0.000000	4.217901	6.466178
C	-1.204241	3.811293	5.890705
C	-1.227674	3.019626	4.739987
C	2.538400	2.538400	4.147890
C	3.019626	1.227674	4.739987
C	2.643663	0.000000	4.147958
C	3.019626	-1.227674	4.739987
C	3.811293	-1.204241	5.890705
C	4.217901	0.000000	6.466178
C	3.811293	1.204241	5.890705
O	1.938505	0.000000	2.994670
C	2.538400	-2.538400	4.147890
C	1.227674	-3.019626	4.739987
C	0.000000	-2.643663	4.147958
C	-1.227674	-3.019626	4.739987
C	-1.204241	-3.811293	5.890705
C	0.000000	-4.217901	6.466178
C	1.204241	-3.811293	5.890705
O	0.000000	-1.938505	2.994670
C	-2.538400	-2.538400	4.147890
C	-3.019626	-1.227674	4.739987
C	-2.643663	0.000000	4.147958
C	-3.019626	1.227674	4.739987
C	-3.811293	1.204241	5.890705
C	-4.217901	0.000000	6.466178
C	-3.811293	-1.204241	5.890705
O	-1.938505	0.000000	2.994670
C	-2.538400	2.538400	4.147890
H	-3.303614	-3.303614	4.323610
H	-2.416660	-2.416660	3.067902
H	3.303614	3.303614	4.323610
H	2.416660	2.416660	3.067902
H	3.303614	-3.303614	4.323610
H	2.416660	-2.416660	3.067902
H	-3.303614	3.303614	4.323610
H	-2.416660	2.416660	3.067902
H	-4.106829	2.148553	6.341524
H	-4.106829	-2.148553	6.341524
H	-4.837543	0.000000	7.357702
H	4.106829	-2.148553	6.341524
H	4.106829	2.148553	6.341524
H	4.837543	0.000000	7.357702
H	-2.148553	-4.106829	6.341524
H	2.148553	-4.106829	6.341524
H	0.000000	-4.837543	7.357702
H	2.148553	4.106829	6.341524
H	-2.148553	4.106829	6.341524

H	0.000000	4.837543	7.357702
H	3.303614	-3.303614	-4.323610
H	2.416660	-2.416660	-3.067902
H	-3.303614	3.303614	-4.323610
H	-2.416660	2.416660	-3.067902
H	-3.303614	-3.303614	-4.323610
H	-2.416660	-2.416660	-3.067902
H	3.303614	3.303614	-4.323610
H	2.416660	2.416660	-3.067902
H	4.106829	2.148553	-6.341524
H	4.106829	-2.148553	-6.341524
H	-4.106829	-2.148553	-6.341524
H	-4.106829	2.148553	-6.341524
H	2.148553	-4.106829	-6.341524
H	-2.148553	-4.106829	-6.341524
H	-2.148553	4.106829	-6.341524
H	2.148553	4.106829	-6.341524
H	4.837543	0.000000	-7.357702
H	-4.837543	0.000000	-7.357702

Table 23: Cartesian coordinates of **(2)** D_{4h} Symmetry X3LYP / SDDAll, spin singlet, equilibrium N−N distance equals 1.283 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.455051
Nb	0.000000	0.000000	-2.455051
N	0.000000	0.000000	-0.641578
N	0.000000	0.000000	0.641578
C	1.232268	3.040675	-4.774687
C	0.000000	2.662601	-4.182752
C	-1.232268	3.040675	-4.774687
C	-1.207683	3.842960	-5.923175
C	0.000000	4.255372	-6.496660
C	1.207683	3.842960	-5.923175
O	-1.949159	0.000000	-3.021978
O	0.000000	1.949159	-3.021978
C	-2.662601	0.000000	-4.182752
C	-3.040675	-1.232268	-4.774687
C	-3.842960	-1.207683	-5.923175
C	-4.255372	0.000000	-6.496660
C	-3.842960	1.207683	-5.923175
C	-3.040675	1.232268	-4.774687
C	-2.555081	-2.555081	-4.187049
C	-1.232268	-3.040675	-4.774687
C	0.000000	-2.662601	-4.182752
C	1.232268	-3.040675	-4.774687
C	1.207683	-3.842960	-5.923175
C	0.000000	-4.255372	-6.496660
C	-1.207683	-3.842960	-5.923175
C	-2.555081	2.555081	-4.187049
O	0.000000	-1.949159	-3.021978
C	2.555081	-2.555081	-4.187049
C	3.040675	-1.232268	-4.774687
C	2.662601	0.000000	-4.182752
C	3.040675	1.232268	-4.774687
C	3.842960	1.207683	-5.923175
C	4.255372	0.000000	-6.496660
C	3.842960	-1.207683	-5.923175
O	1.949159	0.000000	-3.021978
C	2.555081	2.555081	-4.187049
H	0.000000	-4.882513	-7.383728
H	0.000000	4.882513	-7.383728
O	0.000000	1.949159	3.021978
C	0.000000	2.662601	4.182752
C	1.232268	3.040675	4.774687
C	1.207683	3.842960	5.923175
C	0.000000	4.255372	6.496660
C	-1.207683	3.842960	5.923175
C	-1.232268	3.040675	4.774687
C	2.555081	2.555081	4.187049
C	3.040675	1.232268	4.774687
C	2.662601	0.000000	4.182752
C	3.040675	-1.232268	4.774687
C	3.842960	-1.207683	5.923175
C	4.255372	0.000000	6.496660
C	3.842960	1.207683	5.923175
O	1.949159	0.000000	3.021978
C	2.555081	-2.555081	4.187049
C	1.232268	-3.040675	4.774687
C	0.000000	-2.662601	4.182752
C	-1.232268	-3.040675	4.774687
C	-1.207683	-3.842960	5.923175
C	0.000000	-4.255372	6.496660
C	1.207683	-3.842960	5.923175
O	0.000000	-1.949159	3.021978
C	-2.555081	-2.555081	4.187049
C	-3.040675	-1.232268	4.774687
C	-2.662601	0.000000	4.182752
C	-3.040675	1.232268	4.774687
C	-3.842960	1.207683	5.923175

C	-4.255372	0.000000	6.496660
C	-3.842960	-1.207683	5.923175
O	-1.949159	0.000000	3.021978
C	-2.555081	2.555081	4.187049
H	-3.318873	-3.318873	4.378653
H	-2.444939	-2.444939	3.105190
H	3.318873	3.318873	4.378653
H	2.444939	2.444939	3.105190
H	3.318873	-3.318873	4.378653
H	2.444939	-2.444939	3.105190
H	-3.318873	3.318873	4.378653
H	-2.444939	2.444939	3.105190
H	-4.142823	2.151429	6.373144
H	-4.142823	-2.151429	6.373144
H	-4.882513	0.000000	7.383728
H	4.142823	-2.151429	6.373144
H	4.142823	2.151429	6.373144
H	4.882513	0.000000	7.383728
H	-2.151429	-4.142823	6.373144
H	2.151429	-4.142823	6.373144
H	0.000000	-4.882513	7.383728
H	2.151429	4.142823	6.373144
H	-2.151429	4.142823	6.373144
H	0.000000	4.882513	7.383728
H	3.318873	-3.318873	-4.378653
H	2.444939	-2.444939	-3.105190
H	-3.318873	3.318873	-4.378653
H	-2.444939	2.444939	-3.105190
H	-3.318873	-3.318873	-4.378653
H	-2.444939	-2.444939	-3.105190
H	3.318873	3.318873	-4.378653
H	2.444939	2.444939	-3.105190
H	4.142823	2.151429	-6.373144
H	4.142823	-2.151429	-6.373144
H	-4.142823	-2.151429	-6.373144
H	-4.142823	2.151429	-6.373144
H	2.151429	-4.142823	-6.373144
H	-2.151429	-4.142823	-6.373144
H	-2.151429	4.142823	-6.373144
H	2.151429	4.142823	-6.373144
H	4.882513	0.000000	-7.383728
H	-4.882513	0.000000	-7.383728

Table 24: Cartesian coordinates of **(2)** D_{4h} Symmetry GGA Becke Perdew / SDDAll, spin singlet, equilibrium N−N distance equals 1.279 Å

Atom	X	Y	Z
Nb	0.000000	0.000000	2.470198
Nb	0.000000	0.000000	-2.470198
N	0.000000	0.000000	-0.639437
N	0.000000	0.000000	0.639437
C	1.239483	3.049670	-4.773621
C	0.000000	2.668747	-4.177291
C	-1.239483	3.049670	-4.773621
C	-1.214263	3.854424	-5.929153
C	0.000000	4.268643	-6.505858
C	1.214263	3.854424	-5.929153
O	-1.964552	0.000000	-3.004562
O	0.000000	1.964552	-3.004562
C	-2.668747	0.000000	-4.177291
C	-3.049670	-1.239483	-4.773621
C	-3.854424	-1.214263	-5.929153
C	-4.268643	0.000000	-6.505858
C	-3.854424	1.214263	-5.929153
C	-3.049670	1.239483	-4.773621
C	-2.562733	-2.562733	-4.181736
C	-1.239483	-3.049670	-4.773621
C	0.000000	-2.668747	-4.177291
C	1.239483	-3.049670	-4.773621
C	1.214263	-3.854424	-5.929153
C	0.000000	-4.268643	-6.505858
C	-1.214263	-3.854424	-5.929153
C	-2.562733	2.562733	-4.181736
O	0.000000	-1.964552	-3.004562
C	2.562733	-2.562733	-4.181736
C	3.049670	-1.239483	-4.773621
C	2.668747	0.000000	-4.177291
C	3.049670	1.239483	-4.773621
C	3.854424	1.214263	-5.929153
C	4.268643	0.000000	-6.505858
C	3.854424	-1.214263	-5.929153
O	1.964552	0.000000	-3.004562
C	2.562733	2.562733	-4.181736
H	0.000000	-4.900746	-7.400129
H	0.000000	4.900746	-7.400129
O	0.000000	1.964552	3.004562
C	0.000000	2.668747	4.177291
C	1.239483	3.049670	4.773621
C	1.214263	3.854424	5.929153
C	0.000000	4.268643	6.505858
C	-1.214263	3.854424	5.929153

C	-1.239483	3.049670	4.773621
C	2.562733	2.562733	4.181736
C	3.049670	1.239483	4.773621
C	2.668747	0.000000	4.177291
C	3.049670	-1.239483	4.773621
C	3.854424	-1.214263	5.929153
C	4.268643	0.000000	6.505858
C	3.854424	1.214263	5.929153
O	1.964552	0.000000	3.004562
C	2.562733	-2.562733	4.181736
C	1.239483	-3.049670	4.773621
C	0.000000	-2.668747	4.177291
C	-1.239483	-3.049670	4.773621
C	-1.214263	-3.854424	5.929153
C	0.000000	-4.268643	6.505858
C	1.214263	-3.854424	5.929153
O	0.000000	-1.964552	3.004562
C	-2.562733	-2.562733	4.181736
C	-3.049670	-1.239483	4.773621
C	-2.668747	0.000000	4.177291
C	-3.049670	1.239483	4.773621
C	-3.854424	1.214263	5.929153
C	-4.268643	0.000000	6.505858
C	-3.854424	-1.214263	5.929153
O	-1.964552	0.000000	3.004562
C	-2.562733	2.562733	4.181736
H	-3.333500	-3.333500	4.366699
H	-2.444613	-2.444613	3.091834
H	3.333500	3.333500	4.366699
H	2.444613	2.444613	3.091834
H	3.333500	-3.333500	4.366699
H	2.444613	-2.444613	3.091834
H	-3.333500	3.333500	4.366699
H	-2.444613	2.444613	3.091834
H	-4.155710	2.166122	6.382587
H	-4.155710	-2.166122	6.382587
H	-4.900746	0.000000	7.400129
H	4.155710	-2.166122	6.382587
H	4.155710	2.166122	6.382587
H	4.900746	0.000000	7.400129
H	-2.166122	-4.155710	6.382587
H	2.166122	-4.155710	6.382587
H	0.000000	-4.900746	7.400129
H	2.166122	4.155710	6.382587
H	-2.166122	4.155710	6.382587
H	0.000000	4.900746	7.400129
H	3.333500	-3.333500	-4.366699
H	2.444613	-2.444613	-3.091834
H	-3.333500	3.333500	-4.366699
H	-2.444613	2.444613	-3.091834
H	-3.333500	-3.333500	-4.366699
H	-2.444613	-2.444613	-3.091834
H	3.333500	3.333500	-4.366699
H	2.444613	2.444613	-3.091834
H	4.155710	2.166122	-6.382587
H	4.155710	-2.166122	-6.382587
H	-4.155710	-2.166122	-6.382587
H	-4.155710	2.166122	-6.382587
H	2.166122	-4.155710	-6.382587
H	-2.166122	-4.155710	-6.382587
H	-2.166122	4.155710	-6.382587
H	2.166122	4.155710	-6.382587
H	4.900746	0.000000	-7.400129
H	-4.900746	0.000000	-7.400129