10.1071/CH11179_AC

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Accessory Publication

Energetics and Geometries (in Cartesian Co-ordinates) of the doublet state minima

Nb_2Rh
E=-225.371846 a.u.
E+V=-225.370187 a.u.

Nb	0.00000000	1.32858500	0.00000000
Nb	1.27545200	-0.43446800	0.00000000
Rh	-1.16207900	-0.81464000	0.00000000

$NbRh_2$
E=-279.133215 a.u.
E+V=-279.131345 a.u.

Nb	0.00000000	0.00000000	1.16439900
Rh	0.00000000	1.40021900	-0.53044800
Rh	0.00000000	-1.40021900	-0.53044800

Nb_2RhCO
Structure 1
E = -338.896160 a.u.
E+V = -338.889202 a.u.

O	0.07297400	0.08027400	0.04546400
C	0.28604400	0.69648700	4.11921800
Rh	1.53223400	0.06823600	1.07614100
Nb	1.41326200	-0.75428800	3.46188100
Nb	1.69421000	1.57712500	3.09288400

Structure 2
E = -338.902170 a.u.
E+V = -338.894742 a.u.

O	2.983609	-0.000220	0.406525
C	4.035674	-0.002365	0.920274
Rh	1.012088	-0.001605	-0.433375
Nb	-1.139135	1.086069	0.130503
Nb	-1.144447	-1.083918	0.131156

Structure 3
E = -338.908250 a.u.
E+V = -338.901228 a.u.

O	2.821596	0.011618	0.997263
C	3.152798	-0.768755	0.108632
Rh	-1.284277	-0.954729	0.131617
Nb	-0.573136	1.374254	0.044743
Nb	0.970768	-0.216147	-0.399686

Structure 4
E = -338.910810 a.u.
E+V = -338.902985 a.u.

O	2.874858	-0.276197	0.472128
C	3.953614	-0.272318	0.973739
Rh	-1.546687	-0.714273	0.209681
Nb	-0.394301	1.289067	0.022020
Nb	0.952358	-0.411366	-0.486780

Structure 5
E = -338.913210 a.u.
E+V = -338.905860 a.u.

O	-1.289343	1.068332	0.955328
C	-1.805872	-0.284592	1.451353
Rh	1.377907	-0.681742	0.149877
Nb	0.303790	1.234752	-0.208975
Nb	-1.300274	-0.653307	-0.354322

Structure 6
E = -338.932877 a.u.
E+V = -338.925057 a.u.

O	-0.22564900	0.16599100	-0.02223800
C	0.25240300	-0.31243900	1.23179600
Nb	1.98579700	-0.09100400	-0.16454200
Nb	0.95089100	1.90568600	-0.25783100
Rh	1.23220100	1.06388000	2.12256700

Structure 7
E = -338.936345 a.u.
E+V = -338.928222 a.u.

O	0.40321000	0.24424600	-0.01329800
C	1.02702000	0.68647400	4.68593300
Nb	0.36766600	-0.76702100	3.64100900
Nb	0.69513800	1.96365400	3.30034800
Rh	-0.15643800	0.49973300	1.67068600

Structure 8
E = -338.936693 a.u.
E+V = -338.929741 a.u.

O	-0.64786100	-0.00001000	-1.12292200
C	-0.44726900	0.00000100	3.72228500
Rh	0.66881400	0.00000500	2.41413100
Nb	-0.49403000	1.19050200	0.42632200
Nb	-0.49399500	-1.19052500	0.42630800

Structure 9
E = -338.943116 a.u.
E+V = -338.935908 a.u.

C	-0.00104900	0.03850000	0.23688000
O	0.21501200	-0.76715700	3.93735800
Rh	1.56977600	-0.07071200	0.89656800
Nb	1.60423500	0.52689700	3.43907800
Nb	1.65417100	-1.67278800	2.95880700

Structure 10
E = -338.945988 a.u.
E+V = -338.938148 a.u.

C	0.04897200	-0.07748600	0.16430000
O	-0.06376000	0.03743900	3.68204000
Rh	0.75591300	0.03496500	1.80252900
Nb	-1.64226100	0.65968200	2.99381100
Nb	-1.68645600	-0.65461800	0.89176200

Structure 11
E = -338.970060 a.u.
E+V = -338.945558 a.u.

O	-2.365539	0.091566	1.190506
C	-0.445397	-1.789770	-0.075981
Rh	1.186762	-0.916397	0.074632
Nb	-1.476216	-0.112021	-0.303048
Nb	0.700422	1.361873	-0.000040

Structure 12
E = -338.956160 a.u.
E+V = -338.947881 a.u.

Nb	-0.09044400	0.27057200	-0.02434200
Nb	-0.16568200	-0.75194100	1.92028900
Rh	2.19680200	-0.12252100	0.82265100
C	2.22538700	0.36408800	2.61845800
O	1.25770600	0.23980200	3.41159200

Structure 13
E = -338.958640 a.u.
E+V = -338.949748 a.u.

O	-0.747398	-1.206188	1.653052
C	0.070423	-0.239429	1.235176
Rh	1.488434	-0.419197	-0.158684
Nb	-1.264844	-0.660923	-0.398224
Nb	-0.233275	1.391410	0.069085

Structure 14
E = -338.958580 a.u.
E+V = -338.951161 a.u.

O	-2.262623	0.001595	-0.151881
C	-1.541403	0.000904	1.272931
Rh	1.575042	-0.000514	0.059244
Nb	-0.530039	1.187238	-0.110867
Nb	-0.531606	-1.187118	-0.110804

Structure 15
E = -338.980900 a.u.
E+V = -338.955606 a.u.

O	2.575903	0.366945	0.366059
C	1.495456	1.162199	0.280414
Rh	-1.316420	-0.715424	0.093342
Nb	-0.326025	1.485244	-0.083640
Nb	1.049414	-0.941699	-0.131271

Structure 16
E = -338.971706 a.u.
E+V = -338.962373 a.u.

C	0.15000600	-0.00007900	0.09751000
O	-0.24370800	0.00305000	1.21829000
Rh	0.45528500	-0.00434300	-1.71200700
Nb	-1.50761700	1.07979800	-2.94841800
Nb	-1.51570000	-1.07834800	-2.94287900

Structure 17
E = -338.973480 a.u.
E+V = -338.964648 a.u.

O	-2.981780	0.722866	0.000686
C	-1.763792	0.625986	0.000462
Rh	-0.760396	-1.117385	-0.000223
Nb	1.471973	-0.434576	0.000255
Nb	0.202535	1.428319	-0.000211

Structure 18
E = -338.987835 a.u.
E+V = -338.978937 a.u.

C	-0.11459100	-0.54941800	0.29361400
O	-0.73189500	0.53416000	0.75411600
Rh	2.86587700	0.22844500	1.74049800
Nb	1.29539800	1.04799700	0.27104800
Nb	1.66999200	-1.26118500	-0.08703600

Structure 19
E = -338.987450 a.u.
E+V = -338.979516 a.u.

C	0.40563000	-0.66528300	1.16388300
O	0.26330800	-0.44223800	4.59623500
Nb	-0.30729300	0.97912600	1.74324600
Nb	-0.19249200	-1.28165500	2.99515700
Rh	1.24080700	0.98656500	3.49275600

Structure 20
E = -338.990590 a.u.
E+V = -338.983000 a.u.

C	-0.08488400	-0.00692600	0.60991500
O	0.22277100	0.13905200	4.60249400
Nb	-0.29569800	-0.40909200	3.01284600
Nb	0.10840200	1.61578000	1.46136100
Rh	1.45936800	-0.91532900	1.44073400

Structure 21
E = -338.992069 a.u.
E+V = -338.983950 a.u.

O	-0.00006900	0.21041800	-0.08177600
C	0.01425000	-0.11928900	2.85422600
Nb	1.87244000	0.09575600	2.32428200
Nb	-0.25578800	1.19131800	1.44895300
Rh	1.93652400	-0.45040000	0.08317400

Structure 22
E = -339.000648 a.u.
E+V = -338.992708 a.u.

C	0.21438900	0.35682100	0.20714000
O	-0.37174900	0.32367600	3.61791700
Rh	1.69664300	-0.31048600	1.18354200
Nb	1.30687600	0.92156200	3.13983500
Nb	-0.66350300	1.17745800	1.65556600

Structure 23
E = -339.001930 a.u.
E+V = -338.994134 a.u.

O	-1.618421	0.803155	0.994322
C	0.359116	-1.701724	0.373122
Rh	1.569598	-0.310214	0.041709
Nb	-1.283152	-0.861750	-0.154156
Nb	-0.176341	1.294547	-0.140239

Structure 24
E = -339.023370 a.u.
E+V = -339.015228 a.u.

O	1.459697	0.906897	1.139469
C	-0.145182	-1.053381	-0.240882
Rh	-1.890699	-0.381730	0.098162
Nb	1.757466	-0.642425	-0.064580
Nb	0.054119	1.038595	-0.230243

Structure 25
E = -339.032610 a.u.
E+V = -339.024429 a.u.

O	0.27893500	0.82110400	-0.02414600
C	-0.66840500	0.01286100	2.44953000
Nb	0.83646600	-0.58938600	1.26799100
Nb	-1.44139000	0.28047100	0.72909800
Rh	-0.48074400	-2.20141900	0.31738300

Structure 26
E = -339.038163 a.u.
E+V = -339.030163 a.u.

C	1.04460500	-1.14956000	1.61584700
O	1.00971000	-0.30759200	4.35978400
Nb	1.85373100	0.30916900	2.67724300
Nb	-0.32188800	-0.55474900	2.91453000
Rh	-0.07034200	1.68579400	1.71727300

Structure 27
E = -339.052122 a.u.
E+V = -339.043268 a.u.

C	0.67443300	-0.78704500	1.09773200
O	-0.30467700	0.51896300	3.67053800
Nb	1.54869800	0.58151900	0.16845700
Nb	1.14414600	-0.08826900	2.90025500
Rh	2.40929700	1.76601600	2.01123000

$NbRh_2CO$

Structure 28
E = -392.666350 a.u.
E+V = -392.658626 a.u.

O	-3.14236100	-0.16067900	-0.00009600
C	-4.28573800	0.08895700	0.00037400
Rh	-1.03839900	-0.46935700	-0.00007400
Rh	1.74340900	-0.58977800	0.00005100
Nb	0.46653300	1.18079900	-0.00001100

Structure 29
E = -392.673100 a.u.
E+V = -392.665811 a.u.

O	-2.64064700	-0.01299300	-0.29963700
C	-3.67477400	-0.01525900	-0.94310800
Rh	0.81218800	-1.41908500	-0.15709300
Rh	0.79585400	1.42750600	-0.15645200
Nb	-0.71190400	-0.00447400	0.54061600

Structure 30
E = -392.676413 a.u.
E+V = -392.668888 a.u.

Rh	-0.00562000	-0.16408200	-0.04406200
Rh	0.01158300	-0.12820900	2.84818500
Nb	1.85015900	-0.27768900	1.39231200
C	0.35362300	1.24238400	1.38234100
O	1.78311600	1.66595100	1.36683100

Structure 31
E = -392.679210 a.u.
E+V = -392.671770 a.u.

O	-3.16272200	-0.00621600	-0.18881000
C	-2.79706500	-0.00553500	0.99312500
Rh	0.83384900	-1.42870700	0.05714800
Rh	0.82634400	1.43279400	0.05698500
Nb	-0.79572000	-0.00246300	-0.23376300

Structure 32
E = -392.690049 a.u.
E+V = -392.682936 a.u.

Rh	-0.44581700	-0.00930400	0.12091400
Rh	0.14764500	0.01091100	2.72662600
Nb	1.84662900	-0.25020600	1.32331100
O	2.83831500	1.18157300	1.34680500
C	-0.16223300	1.36789500	-0.81038600

Structure 33
E = -392.705174 a.u.
E+V = -392.696291 a.u.

Rh	0.00624500	0.06511200	-0.01817200
Rh	0.00624500	0.06511300	2.81917000
Nb	1.78642300	-0.11203500	1.40049800
C	-1.04317700	0.99836600	1.40049800
O	-1.91669400	1.83844900	1.40049800

Structure 34
E = -392.706525 a.u.
E+V = -392.697885 a.u.

Rh	-0.07467600	0.03372400	-0.02099400
Rh	-0.07786700	0.02734000	2.82244800
Nb	1.55316300	-0.39522400	1.40176600
C	2.94409300	1.20348200	1.40937500
O	3.55311300	2.22269600	1.41266800

Structure 35
E = -392.705809 a.u.
E+V = -392.698316 a.u.

Rh	-0.15372500	0.02347000	-0.26847700
Rh	0.07213900	-0.60830800	2.32429600
Nb	2.15362300	0.34557200	1.34035600
O	1.56098500	1.40498800	0.01451200
C	0.98225700	-1.16572500	0.70691300

Structure 36
E = -392.715980 a.u.
E+V = -392.707041 a.u.

Rh	0.05398700	-0.28255400	0.11220300
Rh	0.04073600	0.03612600	2.91777600
Nb	1.75841900	0.30784000	1.34393800
C	1.64766900	-1.13664400	2.91431700
O	1.94587500	-2.12348800	3.56316800

Structure 37
E = -392.718063 a.u.
E+V = -392.710306 a.u.

Rh	-0.69034500	0.49472900	0.67734600
Rh	-0.16528100	-0.87578000	2.78247100
Nb	1.51455700	0.77740900	1.11778200
C	1.55028500	-0.65606200	2.71513200
O	2.40606200	0.25970000	-0.29023600

Structure 38
E = -392.720920 a.u.
E+V = -392.711660 a.u.

O	3.06882100	0.00077100	0.00102800
C	1.86762100	0.00177600	-0.00025600
Rh	0.31546400	1.29270600	-0.00019400
Rh	0.31771800	-1.29192800	-0.00019400
Nb	-1.56706100	-0.00126400	0.00026200

Structure 39
E = -392.730064 a.u.
E+V = -392.721689 a.u.

Rh	-0.09215500	-0.05423200	-0.24466300
Rh	-0.09215500	-0.05423400	3.04565900
Nb	1.98712600	0.04899600	1.40049900
C	0.15021600	-0.79717400	1.40049800
O	3.15313400	-1.24061500	1.40049900

Structure 40
E = -392.733314 a.u.
E+V = -392.723882 a.u.

Rh	-0.71498900	0.00000000	-0.44416800
Rh	0.18540600	0.00000000	2.33578100
Nb	1.30220900	0.00000000	0.28082700
C	1.53323600	0.00000000	3.58405800
O	2.45525100	0.00000000	4.33136000

Structure 41
E = -392.758849 a.u.
E+V = -392.750547 a.u.

Rh	1.06503700	-1.11916300	-0.26090200
Rh	1.06198600	-1.12005900	3.06201400
Nb	0.78753300	0.64083700	1.39992800
C	1.34619100	-1.77416700	1.40058800
O	-0.82159000	1.30229000	1.40086700

Table S1. Relative energy differences for the global minima of Nb_2Rh and $NbRh_2$ and their respective CO complexes at varying multiplicities.

CLUSTER	**E(S =1/2) (inc. ZPE) (a.u.)**	**ΔE (w.r.t. S =1/2) (eV)**	**E(S = 3/2) (inc. ZPE) (a.u.)**	**ΔE (w.r.t. S =1/2) (eV)**	**E(S = 5/2) (inc. ZPE) (a.u.)**	**ΔE (w.r.t. S = 1/2) (eV)**	**E(S = 7/2) (inc. ZPE) (a.u.)**	**ΔE (w.r.t. S = 1/2) (eV)**
Nb_2Rh	-225.370183	0.00	-225.362613	0.21	-225.342142	0.76	-225.324457	1.24
$NbRh_2$	-279.131345	0.00	-279.102460	0.79	-279.071854	1.62	-279.046627	2.31
Nb_2RhCO	-339.043269	0.00	-339.023089	0.55	-339.005319	1.03	-338.974929	1.86
$NbRh_2CO$	-392.750547	0.00	-392.736535	0.38	-392.689867	1.65	-392.648923	2.77