

*Electronic supplementary information (ESI)*

# Theoretical study on the stability of double-decker type metal phthalocyanines, $M(\text{Pc})_2$ and $M(\text{Pc})_2^+$ ( $M = \text{Ti}, \text{Sn}$ and $\text{Sc}$ ): critical assessment on the performance of density functional

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*Cartesian coordinates for  $M(\text{Pc})_2$  and  $M(\text{Pc})_2^+$  with the PBE1PBE functional*

Ti(Pc) <sub>2</sub> under D <sub>2</sub> symmetry	2
Ti(Pc) <sub>2</sub> under D <sub>4d</sub> symmetry	3
Ti(Pc) <sub>2</sub> <sup>+</sup> under D <sub>2</sub> symmetry	4
Ti(Pc) <sub>2</sub> <sup>+</sup> under D <sub>4d</sub> symmetry	5
Sn(Pc) <sub>2</sub> under D <sub>2</sub> symmetry	6
Sn(Pc) <sub>2</sub> under D <sub>4d</sub> symmetry	7
Sn(Pc) <sub>2</sub> <sup>+</sup> under D <sub>2</sub> symmetry	8
Sn (Pc) <sub>2</sub> <sup>+</sup> under D <sub>4d</sub> symmetry	9
Sc(Pc) <sub>2</sub> under D <sub>2</sub> symmetry	10
Sc(Pc) <sub>2</sub> under D <sub>4d</sub> symmetry	11
Sc(Pc) <sub>2</sub> <sup>+</sup> under D <sub>2</sub> symmetry	12
Sc(Pc) <sub>2</sub> <sup>+</sup> under D <sub>4d</sub> symmetry	13

## Ti(Pc)<sub>2</sub> D<sub>2</sub> symmetry

Ti	0.00000000	0.00000000	0.00000000	H	-6.17412900	3.72176300	2.98263700
N	0.73519300	1.69702400	1.29810100	H	-7.24621500	1.61386000	2.30038100
N	-0.73519300	-1.69702400	1.29810100	N	-0.73519300	1.69702400	-1.29810100
N	1.75651900	-0.76234200	1.03382100	N	0.73519300	-1.69702400	-1.29810100
N	-1.75651900	0.76234200	1.03382100	N	-1.75651900	-0.76234200	-1.03382100
N	3.13025900	1.25801900	1.33475900	N	1.75651900	0.76234200	-1.03382100
N	-3.13025900	-1.25801900	1.33475900	N	-3.13025900	1.25801900	-1.33475900
N	1.24081800	-2.96355000	1.82474400	N	3.13025900	-1.25801900	-1.33475900
N	-1.24081800	2.96355000	1.82474400	N	-1.24081800	-2.96355000	-1.82474400
C	2.09898200	1.97056500	1.53715800	N	1.24081800	2.96355000	-1.82474400
C	0.05195800	2.77255100	1.74597400	C	-2.09898200	1.97056500	-1.53715800
C	2.05220700	-1.94869900	1.53351100	C	-0.05195800	2.77255100	-1.74597400
C	3.01937400	-0.04506600	0.78891200	C	-2.05220700	-1.94869900	-1.53351100
C	-2.09898200	-1.97056500	1.53715800	C	-3.01937400	-0.04506600	-0.78891200
C	-0.05195800	-2.77255100	1.74597400	C	2.09898200	-1.97056500	-1.53715800
C	-2.05220700	1.94869900	1.53351100	C	0.05195800	-2.77255100	-1.74597400
C	-3.01937400	0.04506600	0.78891200	C	2.05220700	1.94869900	-1.53351100
C	2.23579000	3.31796700	2.11634200	C	3.01937400	0.04506600	-0.78891200
C	0.95558500	3.82028400	2.23802300	C	-2.23579000	3.31796700	-2.11634200
C	3.48682500	-2.09486700	1.77965200	C	-0.95558500	3.82028400	-2.23802300
C	4.09287400	-0.92821500	1.35569000	C	-3.48682500	-2.09486700	-1.77965200
C	-2.23579000	-3.31796700	2.11634200	C	-4.09287400	-0.92821500	-1.35569000
C	-0.95558500	-3.82028400	2.23802300	C	2.23579000	-3.31796700	-2.11634200
C	-3.48682500	2.09486700	1.77965200	C	0.95558500	-3.82028400	-2.23802300
C	-4.09287400	0.92821500	1.35569000	C	3.48682500	2.09486700	-1.77965200
C	3.34266000	4.04744000	2.51297300	C	4.09287400	0.92821500	-1.35569000
C	0.70943900	5.07784100	2.76354700	C	-3.34266000	4.04744000	-2.51297300
C	3.11154400	5.31834700	3.03340500	C	-0.70943900	5.07784100	-2.76354700
C	1.81483500	5.82688500	3.15639600	C	-3.11154400	5.31834700	-3.03340500
C	4.20534100	-3.12837000	2.36420200	C	-1.81483500	5.82688500	-3.15639600
C	5.44630600	-0.71588800	1.55135400	C	-4.20534100	-3.12837000	-2.36420200
C	5.57211600	-2.94121100	2.52754400	C	-5.44630600	-0.71588800	-1.55135400
C	6.18073200	-1.74537400	2.13555200	C	-5.57211600	-2.94121100	-2.52754400
C	-3.34266000	-4.04744000	2.51297300	C	-6.18073200	-1.74537400	-2.13555200
C	-0.70943900	-5.07784100	2.76354700	C	3.34266000	-4.04744000	-2.51297300
C	-3.11154400	-5.31834700	3.03340500	C	0.70943900	-5.07784100	-2.76354700
C	-1.81483500	-5.82688500	3.15639600	C	3.11154400	-5.31834700	-3.03340500
C	-4.20534100	3.12837000	2.36420200	C	1.81483500	-5.82688500	-3.15639600
C	-5.44630600	0.71588800	1.55135400	C	4.20534100	3.12837000	-2.36420200
C	-5.57211600	2.94121100	2.52754400	C	5.44630600	0.71588800	-1.55135400
C	-6.18073200	1.74537400	2.13555200	C	5.57211600	2.94121100	-2.52754400
H	4.34276400	3.63911000	2.41591100	C	6.18073200	1.74537400	-2.13555200
H	-0.30366400	5.45322500	2.85730800	H	-4.34276400	3.63911000	-2.41591100
H	3.95201000	5.92805000	3.35139500	H	0.30366400	5.45322500	-2.85730800
H	1.67166000	6.82145800	3.56789200	H	-3.95201000	5.92805000	-3.35139500
H	3.70386000	-4.03401800	2.68731200	H	-1.67166000	6.82145800	-3.56789200
H	5.91261400	0.22306400	1.27456700	H	-3.70386000	-4.03401800	-2.68731200
H	6.17412900	-3.72176300	2.98263700	H	-5.91261400	0.22306400	-1.27456700
H	7.24621500	-1.61386000	2.30038100	H	-6.17412900	-3.72176300	-2.98263700
H	-4.34276400	-3.63911000	2.41591100	H	-7.24621500	-1.61386000	-2.30038100
H	0.30366400	-5.45322500	2.85730800	H	4.34276400	-3.63911000	-2.41591100
H	-3.95201000	-5.92805000	3.35139500	H	-0.30366400	-5.45322500	-2.85730800
H	-1.67166000	-6.82145800	3.56789200	H	3.95201000	-5.92805000	-3.35139500
H	-3.70386000	4.03401800	2.68731200	H	1.67166000	-6.82145800	-3.56789200
H	-5.91261400	-0.22306400	1.27456700	H	3.70386000	4.03401800	-2.68731200
				H	5.91261400	-0.22306400	-1.27456700
				H	6.17412900	3.72176300	-2.98263700
				H	7.24621500	1.61386000	-2.30038100

## Ti(Pc)<sub>2</sub> D<sub>4d</sub> symmetry

Ti	0.00000000	0.00000000	0.00000000	H	-7.27008000	1.23036100	2.63202200
N	0.00000000	1.91849600	1.20048900	H	-7.27008000	-1.23036100	2.63202200
N	0.00000000	-1.91849600	1.20048900	N	-1.35658200	1.35658200	-1.20048900
N	1.91849600	0.00000000	1.20048900	N	1.35658200	-1.35658200	-1.20048900
N	-1.91849600	0.00000000	1.20048900	N	-1.35658200	-1.35658200	-1.20048900
N	2.35426500	2.35426500	1.52051900	N	1.35658200	1.35658200	-1.20048900
N	-2.35426500	-2.35426500	1.52051900	N	-3.32943300	0.00000000	-1.52051900
N	2.35426500	-2.35426500	1.52051900	N	3.32943300	0.00000000	-1.52051900
N	-2.35426500	2.35426500	1.52051900	N	0.00000000	-3.32943300	-1.52051900
C	1.09384600	2.70824600	1.45893800	N	0.00000000	3.32943300	-1.52051900
C	-1.09384600	2.70824600	1.45893800	C	-2.68848500	1.14155300	-1.45893800
C	2.70824600	-1.09384600	1.45893800	C	-1.14155300	2.68848500	-1.45893800
C	2.70824600	1.09384600	1.45893800	C	-1.14155300	-2.68848500	-1.45893800
C	-1.09384600	-2.70824600	1.45893800	C	-2.68848500	-1.14155300	-1.45893800
C	1.09384600	-2.70824600	1.45893800	C	2.68848500	-1.14155300	-1.45893800
C	-2.70824600	1.09384600	1.45893800	C	1.14155300	-2.68848500	-1.45893800
C	-2.70824600	-1.09384600	1.45893800	C	1.14155300	2.68848500	-1.45893800
C	0.69528700	4.06076100	1.78320300	C	2.68848500	1.14155300	-1.45893800
C	-0.69528700	4.06076100	1.78320300	C	-3.36303400	2.37974900	-1.78320300
C	4.06076100	-0.69528700	1.78320300	C	-2.37974900	3.36303400	-1.78320300
C	4.06076100	0.69528700	1.78320300	C	-2.37974900	-3.36303400	-1.78320300
C	-0.69528700	-4.06076100	1.78320300	C	-3.36303400	-2.37974900	-1.78320300
C	0.69528700	-4.06076100	1.78320300	C	3.36303400	-2.37974900	-1.78320300
C	-4.06076100	0.69528700	1.78320300	C	2.37974900	-3.36303400	-1.78320300
C	-4.06076100	-0.69528700	1.78320300	C	2.37974900	3.36303400	-1.78320300
C	1.42251600	5.20398700	2.09827300	C	3.36303400	2.37974900	-1.78320300
C	-1.42251600	5.20398700	2.09827300	C	-4.68564500	2.67390400	-2.09827300
C	0.70254300	6.35188700	2.39225600	C	-2.67390400	4.68564500	-2.09827300
C	-0.70254300	6.35188700	2.39225600	C	-4.98823600	3.99469000	-2.39225600
C	5.20398700	-1.42251600	2.09827300	C	-3.99469000	4.98823600	-2.39225600
C	5.20398700	1.42251600	2.09827300	C	-2.67390400	-4.68564500	-2.09827300
C	6.35188700	-0.70254300	2.39225600	C	-4.68564500	-2.67390400	-2.09827300
C	6.35188700	0.70254300	2.39225600	C	-3.99469000	-4.98823600	-2.39225600
C	-1.42251600	-5.20398700	2.09827300	C	-4.98823600	-3.99469000	-2.39225600
C	1.42251600	-5.20398700	2.09827300	C	4.68564500	-2.67390400	-2.09827300
C	-0.70254300	-6.35188700	2.39225600	C	2.67390400	-4.68564500	-2.09827300
C	0.70254300	-6.35188700	2.39225600	C	4.98823600	-3.99469000	-2.39225600
C	-5.20398700	1.42251600	2.09827300	C	3.99469000	4.98823600	-2.39225600
C	-5.20398700	-1.42251600	2.09827300	H	-5.44173500	1.89641800	-2.10538000
C	-6.35188700	0.70254300	2.39225600	H	-1.89641800	5.44173500	-2.10538000
C	-6.35188700	-0.70254300	2.39225600	H	-6.01072000	4.27072600	-2.63202200
H	2.50691700	5.18885800	2.10538000	H	-4.27072600	6.01072000	-2.63202200
H	-2.50691700	5.18885800	2.10538000	H	-1.89641800	-5.44173500	-2.10538000
H	1.23036100	7.27008000	2.63202200	H	-5.44173500	-1.89641800	-2.10538000
H	-1.23036100	7.27008000	2.63202200	H	-4.27072600	-6.01072000	-2.63202200
H	5.18885800	-2.50691700	2.10538000	H	-6.01072000	-4.27072600	-2.63202200
H	5.18885800	2.50691700	2.10538000	H	5.44173500	-1.89641800	-2.10538000
H	7.27008000	-1.23036100	2.63202200	H	1.89641800	-5.44173500	-2.10538000
H	7.27008000	1.23036100	2.63202200	H	6.01072000	-4.27072600	-2.63202200
H	-2.50691700	-5.18885800	2.10538000	H	4.27072600	-6.01072000	-2.63202200
H	2.50691700	-5.18885800	2.10538000	H	1.89641800	5.44173500	-2.10538000
H	-1.23036100	-7.27008000	2.63202200	H	5.44173500	1.89641800	-2.10538000
H	1.23036100	-7.27008000	2.63202200	H	4.27072600	6.01072000	-2.63202200
H	-5.18885800	2.50691700	2.10538000	H	6.01072000	4.27072600	-2.63202200
H	-5.18885800	-2.50691700	2.10538000				

## Ti(Pc)<sub>2</sub><sup>+</sup> D<sub>2</sub> symmetry

Ti	0.00000000	0.00000000	0.00000000	H	-6.20599000	3.68202500	2.94816200
N	0.73396900	1.71789900	1.26147300	H	-7.24876300	1.55161300	2.30062200
N	-0.73396900	-1.71789900	1.26147300	N	-0.73396900	1.71789900	-1.26147300
N	1.75238900	-0.73065100	1.06319400	N	0.73396900	-1.71789900	-1.26147300
N	-1.75238900	0.73065100	1.06319400	N	-1.75238900	-0.73065100	-1.06319400
N	3.11960700	1.29789100	1.28531000	N	1.75238900	0.73065100	-1.06319400
N	-3.11960700	-1.29789100	1.28531000	N	-3.11960700	1.29789100	-1.28531000
N	1.25633700	-2.95588500	1.79999600	N	3.11960700	-1.29789100	-1.28531000
N	-1.25633700	2.95588500	1.79999600	N	-1.25633700	-2.95588500	-1.79999600
C	2.08745600	2.02470300	1.47462500	N	1.25633700	2.95588500	-1.79999600
C	0.03862100	2.80053600	1.69982500	C	-2.08745600	2.02470300	-1.47462500
C	2.06494200	-1.93497500	1.53647300	C	-0.03862100	2.80053600	-1.69982500
C	2.99801400	-0.01804100	0.84420100	C	-2.06494200	-1.93497500	-1.53647300
C	-2.08745600	-2.02470300	1.47462500	C	-2.99801400	-0.01804100	-0.84420100
C	-0.03862100	-2.80053600	1.69982500	C	2.08745600	-2.02470300	-1.47462500
C	-2.06494200	1.93497500	1.53647300	C	0.03862100	-2.80053600	-1.69982500
C	-2.99801400	0.01804100	0.84420100	C	2.06494200	1.93497500	-1.53647300
C	2.21807400	3.38741100	2.00626300	C	2.99801400	0.01804100	-0.84420100
C	0.93041700	3.87162900	2.14570600	C	-2.21807400	3.38741100	-2.00626300
C	3.49535100	-2.07204800	1.78074800	C	-0.93041700	3.87162900	-2.14570600
C	4.08789300	-0.88805100	1.38164900	C	-3.49535100	-2.07204800	-1.78074800
C	-2.21807400	-3.38741100	2.00626300	C	4.08789300	0.88805100	-1.38164900
C	-0.93041700	-3.87162900	2.14570600	C	-2.21807400	-3.38741100	-2.00626300
C	-3.49535100	2.07204800	1.78074800	C	0.93041700	-3.87162900	-2.14570600
C	-4.08789300	0.88805100	1.38164900	C	3.49535100	2.07204800	-1.78074800
C	3.32151400	4.14196000	2.36264100	C	4.08789300	0.88805100	-1.38164900
C	0.67382400	5.13664600	2.64830200	C	-2.21807400	-3.38741100	-2.00626300
C	3.07811900	5.42122200	2.85790600	C	-0.93041700	-3.87162900	-2.14570600
C	1.77630800	5.91121200	2.99819300	C	-3.49535100	-2.07204800	-1.78074800
C	4.22833900	-3.10738800	2.34569200	C	4.08789300	0.88805100	-1.38164900
C	5.43813500	-0.65892300	1.57372000	C	-2.21807400	-3.38741100	-2.00626300
C	5.59233400	-2.90277200	2.50818200	C	-0.93041700	-3.87162900	-2.14570600
C	6.18499300	-1.69201700	2.13605500	C	3.49535100	2.07204800	-1.78074800
C	-3.32151400	-4.14196000	2.36264100	C	4.08789300	0.88805100	-1.38164900
C	-0.67382400	-5.13664600	2.64830200	C	-2.21807400	-3.38741100	-2.00626300
C	-3.07811900	-5.42122200	2.85790600	C	-0.93041700	-3.87162900	-2.14570600
C	-1.77630800	-5.91121200	2.99819300	C	-3.49535100	-2.07204800	-1.78074800
C	-4.22833900	3.10738800	2.34569200	C	4.08789300	0.88805100	-1.38164900
C	-5.43813500	0.65892300	1.57372000	C	-2.21807400	-3.38741100	-2.00626300
C	-5.59233400	2.90277200	2.50818200	C	-0.93041700	-3.87162900	-2.14570600
C	-6.18499300	1.69201700	2.13605500	C	3.49535100	2.07204800	-1.78074800
H	4.32743900	3.75091100	2.25825700	C	4.08789300	0.88805100	-1.38164900
H	-0.34139600	5.50060800	2.75965000	C	-2.21807400	-3.38741100	-2.00626300
H	3.91397400	6.05138400	3.14451400	C	-0.93041700	-3.87162900	-2.14570600
H	1.62621900	6.91150800	3.39124600	C	3.49535100	2.07204800	-1.78074800
H	3.74345100	-4.02567400	2.65740400	C	4.08789300	0.88805100	-1.38164900
H	5.89313200	0.28927800	1.31112400	C	-2.21807400	-3.38741100	-2.00626300
H	6.20599000	-3.68202500	2.94816200	C	-0.93041700	-3.87162900	-2.14570600
H	7.24876300	-1.55161300	2.30062200	C	3.49535100	2.07204800	-1.78074800
H	-4.32743900	-3.75091100	2.25825700	C	4.08789300	0.88805100	-1.38164900
H	0.34139600	-5.50060800	2.75965000	C	-2.21807400	-3.38741100	-2.00626300
H	-3.91397400	-6.05138400	3.14451400	C	-0.93041700	-3.87162900	-2.14570600
H	-1.62621900	-6.91150800	3.39124600	C	3.49535100	2.07204800	-1.78074800
H	-3.74345100	4.02567400	2.65740400	C	4.08789300	0.88805100	-1.38164900
H	-5.89313200	-0.28927800	1.31112400	C	-2.21807400	-3.38741100	-2.00626300

**Ti(Pc)<sub>2</sub><sup>+</sup> D<sub>4d</sub> symmetry**

Ti	0.00000000	0.00000000	0.00000000	H	-7.27374900	1.22851000	2.58995200
N	0.00000000	1.91164700	1.18719700	H	-7.27374900	-1.22851000	2.58995200
N	0.00000000	-1.91164700	1.18719700	N	-1.35173800	1.35173800	-1.18719700
N	1.91164700	0.00000000	1.18719700	N	1.35173800	-1.35173800	-1.18719700
N	-1.91164700	0.00000000	1.18719700	N	-1.35173800	-1.35173800	-1.18719700
N	2.35450400	2.35450400	1.49105200	N	1.35173800	1.35173800	-1.18719700
N	-2.35450400	-2.35450400	1.49105200	N	-3.32977100	0.00000000	-1.49105200
N	2.35450400	-2.35450400	1.49105200	N	3.32977100	0.00000000	-1.49105200
N	-2.35450400	2.35450400	1.49105200	N	0.00000000	-3.32977100	-1.49105200
C	1.09313600	2.70682300	1.43273100	N	0.00000000	3.32977100	-1.49105200
C	-1.09313600	2.70682300	1.43273100	C	-2.68697700	1.14104900	-1.43273100
C	2.70682300	-1.09313600	1.43273100	C	-1.14104900	2.68697700	-1.43273100
C	2.70682300	1.09313600	1.43273100	C	-1.14104900	-2.68697700	-1.43273100
C	-1.09313600	-2.70682300	1.43273100	C	-2.68697700	-1.14104900	-1.43273100
C	1.09313600	-2.70682300	1.43273100	C	2.68697700	-1.14104900	-1.43273100
C	-2.70682300	1.09313600	1.43273100	C	1.14104900	-2.68697700	-1.43273100
C	-2.70682300	-1.09313600	1.43273100	C	1.14104900	2.68697700	-1.43273100
C	0.69455200	4.06552600	1.74878700	C	2.68697700	1.14104900	-1.43273100
C	-0.69455200	4.06552600	1.74878700	C	-3.36588300	2.38363800	-1.74878700
C	4.06552600	-0.69455200	1.74878700	C	-2.38363800	3.36588300	-1.74878700
C	4.06552600	0.69455200	1.74878700	C	-2.38363800	-3.36588300	-1.74878700
C	-0.69455200	-4.06552600	1.74878700	C	-3.36588300	-2.38363800	-1.74878700
C	0.69455200	-4.06552600	1.74878700	C	3.36588300	-2.38363800	-1.74878700
C	-4.06552600	0.69455200	1.74878700	C	2.38363800	-3.36588300	-1.74878700
C	-4.06552600	-0.69455200	1.74878700	C	2.38363800	3.36588300	-1.74878700
C	1.42360700	5.20532100	2.05955400	C	3.36588300	2.38363800	-1.74878700
C	-1.42360700	5.20532100	2.05955400	C	-4.68736000	2.67407500	-2.05955400
C	0.70098200	6.35611800	2.35010900	C	-2.67407500	4.68736000	-2.05955400
C	-0.70098200	6.35611800	2.35010900	C	-4.99012300	3.99878500	-2.35010900
C	5.20532100	-1.42360700	2.05955400	C	-3.99878500	4.99012300	-2.35010900
C	5.20532100	1.42360700	2.05955400	C	-2.67407500	-4.68736000	-2.05955400
C	6.35611800	-0.70098200	2.35010900	C	-4.68736000	-2.67407500	-2.05955400
C	6.35611800	0.70098200	2.35010900	C	-3.99878500	-4.99012300	-2.35010900
C	-1.42360700	-5.20532100	2.05955400	C	-4.99012300	-3.99878500	-2.35010900
C	1.42360700	-5.20532100	2.05955400	C	4.68736000	-2.67407500	-2.05955400
C	-0.70098200	-6.35611800	2.35010900	C	2.67407500	-4.68736000	-2.05955400
C	0.70098200	-6.35611800	2.35010900	C	4.99012300	-3.99878500	-2.35010900
C	-5.20532100	1.42360700	2.05955400	C	3.99878500	4.99012300	-2.35010900
C	-5.20532100	-1.42360700	2.05955400	C	4.99012300	3.99878500	-2.35010900
C	-6.35611800	0.70098200	2.35010900	H	-5.44417200	1.89777900	-2.07184000
C	-6.35611800	-0.70098200	2.35010900	H	-1.89777900	5.44417200	-2.07184000
H	2.50767800	5.19154300	2.07184000	H	-6.01200500	4.27462900	-2.58995200
H	-2.50767800	5.19154300	2.07184000	H	-4.27462900	6.01200500	-2.58995200
H	1.22851000	7.27374900	2.58995200	H	-1.89777900	-5.44417200	-2.07184000
H	-1.22851000	7.27374900	2.58995200	H	-5.44417200	-1.89777900	-2.07184000
H	5.19154300	-2.50767800	2.07184000	H	-4.27462900	-6.01200500	-2.58995200
H	5.19154300	2.50767800	2.07184000	H	-6.01200500	-4.27462900	-2.58995200
H	7.27374900	-1.22851000	2.58995200	H	5.44417200	-1.89777900	-2.07184000
H	7.27374900	1.22851000	2.58995200	H	1.89777900	-5.44417200	-2.07184000
H	-2.50767800	-5.19154300	2.07184000	H	6.01200500	-4.27462900	-2.58995200
H	2.50767800	-5.19154300	2.07184000	H	4.27462900	-6.01200500	-2.58995200
H	-1.22851000	-7.27374900	2.58995200	H	1.89777900	5.44417200	-2.07184000
H	1.22851000	-7.27374900	2.58995200	H	5.44417200	1.89777900	-2.07184000
H	-5.19154300	2.50767800	2.07184000	H	4.27462900	6.01200500	-2.58995200
H	-5.19154300	-2.50767800	2.07184000	H	6.01200500	4.27462900	-2.58995200

## Sn(Pc)<sub>2</sub> D<sub>2</sub> symmetry

Sn	0.00000000	0.00000000	0.00000000	H	-6.22203400	3.68795800	3.02519200
N	0.75320400	1.71727700	1.36832500	H	-7.28489200	1.59143200	2.29381300
N	-0.75320400	-1.71727700	1.36832500	N	-0.75320400	1.71727700	-1.36832500
N	1.79704700	-0.76352900	1.08295300	N	0.75320400	-1.71727700	-1.36832500
N	-1.79704700	0.76352900	1.08295300	N	-1.79704700	-0.76352900	-1.08295300
N	3.14741400	1.27819500	1.33187400	N	1.79704700	0.76352900	-1.08295300
N	-3.14741400	-1.27819500	1.33187400	N	-3.14741400	1.27819500	-1.33187400
N	1.24733400	-2.93451000	1.93792800	N	3.14741400	-1.27819500	-1.33187400
N	-1.24733400	2.93451000	1.93792800	N	-1.24733400	-2.93451000	-1.93792800
C	2.12049600	1.99261800	1.56579000	N	1.24733400	2.93451000	-1.93792800
C	0.05219100	2.76906200	1.84105200	C	-2.12049600	1.99261800	-1.56579000
C	2.07688200	-1.94220600	1.60500800	C	-0.05219100	2.76906200	-1.84105200
C	3.04267700	-0.03940000	0.79773600	C	-2.07688200	-1.94220600	-1.60500800
C	-2.12049600	-1.99261800	1.56579000	C	-3.04267700	-0.03940000	-0.79773600
C	-0.05219100	-2.76906200	1.84105200	C	2.12049600	-1.99261800	-1.56579000
C	-2.07688200	1.94220600	1.60500800	C	0.05219100	-2.76906200	-1.84105200
C	-3.04267700	0.03940000	0.79773600	C	2.07688200	1.94220600	-1.60500800
C	2.24781100	3.33853500	2.15581400	C	3.04267700	0.03940000	-0.79773600
C	0.96050900	3.81911100	2.32651100	C	-2.12049600	3.33853500	-2.15581400
C	3.51840400	-2.08322800	1.82552500	C	-0.96050900	3.81911100	-2.32651100
C	4.12038500	-0.92190200	1.36885000	C	-3.51840400	-2.08322800	-1.82552500
C	-2.24781100	-3.33853500	2.15581400	C	-4.12038500	-0.92190200	-1.36885000
C	-0.96050900	-3.81911100	2.32651100	C	2.24781100	-3.33853500	-2.15581400
C	-3.51840400	2.08322800	1.82552500	C	0.96050900	-3.81911100	-2.32651100
C	-4.12038500	0.92190200	1.36885000	C	3.51840400	2.08322800	-1.82552500
C	3.35281700	4.08223600	2.52941700	C	4.12038500	0.92190200	-1.36885000
C	0.71423800	5.06451300	2.87935800	C	-3.35281700	4.08223600	-2.52941700
C	3.11873400	5.34134800	3.07749800	C	-0.71423800	5.06451300	-2.87935800
C	1.81925500	5.82595600	3.25013800	C	-3.11873400	5.34134800	-3.07749800
C	4.24591400	-3.10447700	2.41900600	C	-1.81925500	5.82595600	-3.25013800
C	5.47585000	-0.70930000	1.54727800	C	-4.24591400	-3.10447700	-2.41900600
C	5.61506300	-2.91565700	2.56272300	C	-5.47585000	-0.70930000	-1.54727800
C	6.21793900	-1.72739900	2.14268900	C	-5.61506300	-2.91565700	-2.56272300
C	-3.35281700	-4.08223600	2.52941700	C	-6.21793900	-1.72739900	-2.14268900
C	-0.71423800	-5.06451300	2.87935800	C	3.35281700	-4.08223600	-2.52941700
C	-3.11873400	-5.34134800	3.07749800	C	0.71423800	-5.06451300	-2.87935800
C	-1.81925500	-5.82595600	3.25013800	C	3.11873400	-5.34134800	-3.07749800
C	-4.24591400	3.10447700	2.41900600	C	1.81925500	-5.82595600	-3.25013800
C	-5.47585000	0.70930000	1.54727800	C	4.24591400	3.10447700	-2.41900600
C	-5.61506300	2.91565700	2.56272300	C	5.47585000	0.70930000	-1.54727800
C	-6.21793900	1.72739900	2.14268900	C	5.61506300	2.91565700	-2.56272300
H	4.35594800	3.69226700	2.39453300	C	6.21793900	1.72739900	-2.14268900
H	-0.30122600	5.42215600	3.01038400	H	-4.35594800	3.69226700	-2.39453300
H	3.95938800	5.95946000	3.37825900	H	0.30122600	5.42215600	-3.01038400
H	1.67283900	6.81131100	3.68212100	H	-3.95938800	5.95946000	-3.37825900
H	3.74800500	-4.00343600	2.76579000	H	-1.67283900	6.81131100	-3.68212100
H	5.93923300	0.22503900	1.25081400	H	-3.74800500	-4.00343600	-2.76579000
H	6.22203400	-3.68795800	3.02519200	H	-5.93923300	0.22503900	-1.25081400
H	7.28489200	-1.59143200	2.29381300	H	-6.22203400	-3.68795800	-3.02519200
H	-4.35594800	-3.69226700	2.39453300	H	-7.28489200	-1.59143200	-2.29381300
H	0.30122600	-5.42215600	3.01038400	H	4.35594800	-3.69226700	-2.39453300
H	-3.95938800	-5.95946000	3.37825900	H	-0.30122600	-5.42215600	-3.01038400
H	-1.67283900	-6.81131100	3.68212100	H	3.95938800	-5.95946000	-3.37825900
H	-3.74800500	4.00343600	2.76579000	H	1.67283900	-6.81131100	-3.68212100
H	-5.93923300	-0.22503900	1.25081400	H	3.74800500	4.00343600	-2.76579000
				H	5.93923300	-0.22503900	-1.25081400
				H	6.22203400	3.68795800	-3.02519200
				H	7.28489200	1.59143200	-2.29381300

## Sn(Pc)<sub>2</sub> D<sub>4d</sub> symmetry

Sn	0.00000000	0.00000000	0.00000000	H	7.31303500	1.23044700	2.60144900
N	0.00000000	1.94734700	1.27010200	H	7.31303500	-1.23044700	2.60144900
N	0.00000000	-1.94734700	1.27010200	N	1.37698200	1.37698200	-1.27010200
N	-1.94734700	0.00000000	1.27010200	N	-1.37698200	-1.37698200	-1.27010200
N	1.94734700	0.00000000	1.27010200	N	1.37698200	-1.37698200	-1.27010200
N	-2.36256300	2.36256300	1.56153900	N	-1.37698200	1.37698200	-1.27010200
N	2.36256300	-2.36256300	1.56153900	N	3.34116900	0.00000000	-1.56153900
N	-2.36256300	-2.36256300	1.56153900	N	-3.34116900	0.00000000	-1.56153900
N	2.36256300	2.36256300	1.56153900	N	0.00000000	-3.34116900	-1.56153900
C	-1.10197100	2.73039500	1.50432400	N	0.00000000	3.34116900	-1.56153900
C	1.10197100	-2.73039500	1.50432400	C	2.70989200	1.15147000	-1.50432400
C	-2.73039500	-1.10197100	1.50432400	C	-2.70989200	-1.15147000	-1.50432400
C	2.73039500	1.10197100	1.50432400	C	1.15147000	-2.70989200	-1.50432400
C	1.10197100	2.73039500	1.50432400	C	-1.15147000	2.70989200	-1.50432400
C	-1.10197100	-2.73039500	1.50432400	C	1.15147000	2.70989200	-1.50432400
C	-2.73039500	1.10197100	1.50432400	C	-1.15147000	-2.70989200	-1.50432400
C	2.73039500	-1.10197100	1.50432400	C	2.70989200	-1.15147000	-1.50432400
C	-0.69712000	4.08834400	1.80594100	C	-2.70989200	1.15147000	-1.50432400
C	0.69712000	4.08834400	1.80594100	C	3.38383400	2.39795800	-1.80594100
C	-1.42170400	5.23820200	2.10096200	C	2.39795800	3.38383400	-1.80594100
C	1.42170400	5.23820200	2.10096200	C	4.70926500	2.69867100	-2.10096200
C	-0.70216400	6.39132400	2.37669800	C	2.69867100	4.70926500	-2.10096200
C	0.70216400	6.39132400	2.37669800	C	5.01585400	4.02284400	-2.37669800
H	-2.50618200	5.22372200	2.10756100	C	4.02284400	5.01585400	-2.37669800
H	2.50618200	5.22372200	2.10756100	H	5.46586700	1.92159000	-2.10756100
H	-1.23044700	7.31303500	2.60144900	H	1.92159000	5.46586700	-2.10756100
H	1.23044700	7.31303500	2.60144900	H	6.04115400	4.30103900	-2.60144900
C	0.69712000	-4.08834400	1.80594100	H	4.30103900	6.04115400	-2.60144900
C	-0.69712000	-4.08834400	1.80594100	C	-3.38383400	-2.39795800	-1.80594100
C	1.42170400	-5.23820200	2.10096200	C	-2.39795800	-3.38383400	-1.80594100
C	-1.42170400	-5.23820200	2.10096200	C	-4.70926500	-2.69867100	-2.10096200
C	0.70216400	-6.39132400	2.37669800	C	-2.69867100	-4.70926500	-2.10096200
C	-0.70216400	-6.39132400	2.37669800	C	-5.01585400	-4.02284400	-2.37669800
H	2.50618200	-5.22372200	2.10756100	C	-4.02284400	-5.01585400	-2.37669800
H	-2.50618200	-5.22372200	2.10756100	H	-5.46586700	-1.92159000	-2.10756100
H	1.23044700	-7.31303500	2.60144900	H	-1.92159000	-5.46586700	-2.10756100
H	-1.23044700	-7.31303500	2.60144900	H	-6.04115400	-4.30103900	-2.60144900
C	-4.08834400	-0.69712000	1.80594100	H	-4.30103900	-6.04115400	-2.60144900
C	-4.08834400	0.69712000	1.80594100	C	2.39795800	-3.38383400	-1.80594100
C	-5.23820200	-1.42170400	2.10096200	C	3.38383400	-2.39795800	-1.80594100
C	-5.23820200	1.42170400	2.10096200	C	2.69867100	-4.70926500	-2.10096200
C	-6.39132400	-0.70216400	2.37669800	C	4.70926500	-2.69867100	-2.10096200
C	-6.39132400	0.70216400	2.37669800	C	4.02284400	-5.01585400	-2.37669800
H	-5.22372200	-2.50618200	2.10756100	H	1.92159000	-5.46586700	-2.10756100
H	-5.22372200	2.50618200	2.10756100	H	5.46586700	-1.92159000	-2.10756100
H	-7.31303500	-1.23044700	2.60144900	H	4.30103900	-6.04115400	-2.60144900
H	-7.31303500	1.23044700	2.60144900	H	6.04115400	-4.30103900	-2.60144900
C	4.08834400	0.69712000	1.80594100	C	-2.39795800	3.38383400	-1.80594100
C	4.08834400	-0.69712000	1.80594100	C	-3.38383400	2.39795800	-1.80594100
C	5.23820200	1.42170400	2.10096200	C	-2.69867100	4.70926500	-2.10096200
C	5.23820200	-1.42170400	2.10096200	C	-4.70926500	2.69867100	-2.10096200
C	6.39132400	0.70216400	2.37669800	C	-4.02284400	5.01585400	-2.37669800
C	6.39132400	-0.70216400	2.37669800	H	-1.92159000	5.46586700	-2.10756100
H	5.22372200	2.50618200	2.10756100	H	-5.46586700	1.92159000	-2.10756100
H	5.22372200	-2.50618200	2.10756100	H	-4.30103900	6.04115400	-2.60144900
				H	-6.04115400	4.30103900	-2.60144900

## Sn(Pc)<sub>2</sub><sup>+</sup> D<sub>2</sub> symmetry

Sn	0.00000000	0.00000000	0.00000000	H	-6.33736400	3.96791300	2.24191100
N	0.73570600	1.78117600	1.24719600	H	-7.29078400	1.70323800	2.21377100
N	-0.73570600	-1.78117600	1.24719600	N	-0.73570600	1.78117600	-1.24719600
N	1.79691200	-0.74819400	1.21713300	N	0.73570600	-1.78117600	-1.24719600
N	-1.79691200	0.74819400	1.21713300	N	-1.79691200	-0.74819400	-1.21713300
N	3.09602100	1.28260800	1.46191000	N	1.79691200	0.74819400	-1.21713300
N	-3.09602100	-1.28260800	1.46191000	N	-3.09602100	1.28260800	-1.46191000
N	1.27874200	-3.09518400	1.47108300	N	3.09602100	-1.28260800	-1.46191000
N	-1.27874200	3.09518400	1.47108300	N	-1.27874200	-3.09518400	-1.47108300
C	2.07050200	2.09263900	1.43201100	N	1.27874200	3.09518400	-1.47108300
C	0.02357000	2.93059500	1.45114700	C	-2.07050200	2.09263900	-1.43201100
C	2.10847300	-2.06288500	1.39577400	C	-0.02357000	2.93059500	-1.45114700
C	2.96539100	-0.02986000	1.36679400	C	-2.10847300	-2.06288500	-1.39577400
C	-2.07050200	-2.09263900	1.43201100	C	-2.96539100	-0.02986000	-1.36679400
C	-0.02357000	-2.93059500	1.45114700	C	2.07050200	-2.09263900	-1.43201100
C	-2.10847300	2.06288500	1.39577400	C	0.02357000	-2.93059500	-1.45114700
C	-2.96539100	0.02986000	1.36679400	C	2.10847300	2.06288500	-1.39577400
C	2.21465000	3.51478100	1.71792200	C	2.96539100	0.02986000	-1.36679400
C	0.92831700	4.04265600	1.73226200	C	-2.21465000	3.51478100	-1.71792200
C	3.53555600	-2.21718100	1.62138400	C	-0.92831700	4.04265600	-1.73226200
C	4.07592900	-0.93102100	1.60425900	C	-3.53555600	-2.21718100	-1.62138400
C	-2.21465000	-3.51478100	1.71792200	C	-4.07592900	-0.93102100	-1.60425900
C	-0.92831700	-4.04265600	1.73226200	C	2.21465000	-3.51478100	-1.71792200
C	-3.53555600	2.21718100	1.62138400	C	0.92831700	-4.04265600	-1.73226200
C	-4.07592900	0.93102100	1.60425900	C	3.53555600	2.21718100	-1.62138400
C	3.32499300	4.30147100	1.97675700	C	4.07592900	0.93102100	-1.60425900
C	0.69393000	5.37926900	2.00880500	C	-3.32499300	4.30147100	-1.97675700
C	3.09973200	5.65088600	2.23891100	C	-0.69393000	5.37926900	-2.00880500
C	1.80613900	6.18110900	2.25552200	C	-3.09973200	5.65088600	-2.23891100
C	4.32380600	-3.33409800	1.85744000	C	-1.80613900	6.18110900	-2.25552200
C	5.42905800	-0.71216300	1.82384900	C	-4.32380600	-3.33409800	-1.85744000
C	5.68332800	-3.12146800	2.05881300	C	-5.42905800	-0.71216300	-1.82384900
C	6.22656300	-1.83034000	2.04270000	C	-5.68332800	-3.12146800	-2.05881300
C	-3.32499300	-4.30147100	1.97675700	C	-6.22656300	-1.83034000	-2.04270000
C	-0.69393000	-5.37926900	2.00880500	C	3.32499300	-4.30147100	-1.97675700
C	-3.09973200	-5.65088600	2.23891100	C	0.69393000	-5.37926900	-2.00880500
C	-1.80613900	-6.18110900	2.25552200	C	3.09973200	-5.65088600	-2.23891100
C	-4.32380600	3.33409800	1.85744000	C	1.80613900	-6.18110900	-2.25552200
C	-5.42905800	0.71216300	1.82384900	C	4.32380600	3.33409800	-1.85744000
C	-5.68332800	3.12146800	2.05881300	C	5.42905800	0.71216300	-1.82384900
C	-6.22656300	1.83034000	2.04270000	C	5.68332800	3.12146800	-2.05881300
H	4.32336000	3.87847300	1.97339300	C	6.22656300	1.83034000	-2.04270000
H	-0.31455500	5.77707700	2.03092500	H	-4.32336000	3.87847300	-1.97339300
H	3.94197400	6.30455100	2.44192600	H	0.31455500	5.77707700	-2.03092500
H	1.66899300	7.23572500	2.47165800	H	-3.94197400	6.30455100	-2.44192600
H	3.89019700	-4.32761600	1.88261800	H	-1.66899300	7.23572500	-2.47165800
H	5.84006800	0.29125200	1.82338800	H	-3.89019700	-4.32761600	-1.88261800
H	6.33736400	-3.96791300	2.24191100	H	-5.84006800	0.29125200	-1.82338800
H	7.29078400	-1.70323800	2.21377100	H	-6.33736400	-3.96791300	-2.24191100
H	-4.32336000	-3.87847300	1.97339300	H	-7.29078400	-1.70323800	-2.21377100
H	0.31455500	-5.77707700	2.03092500	H	4.32336000	-3.87847300	-1.97339300
H	-3.94197400	-6.30455100	2.44192600	H	-0.31455500	-5.77707700	-2.03092500
H	-1.66899300	-7.23572500	2.47165800	H	3.94197400	-6.30455100	-2.44192600
H	-3.89019700	4.32761600	1.88261800	H	1.66899300	-7.23572500	-2.47165800
H	-5.84006800	-0.29125200	1.82338800	H	3.89019700	4.32761600	-1.88261800
				H	5.84006800	-0.29125200	-1.82338800
				H	6.33736400	3.96791300	-2.24191100
				H	7.29078400	1.70323800	-2.21377100



## Sn(Pc)<sub>2</sub><sup>+</sup> D<sub>4d</sub> symmetry

Sn	0.00000000	0.00000000	0.00000000	H	-7.31838800	1.22861500	2.55020500
N	0.00000000	1.94106200	1.25588500	H	-7.31838800	-1.22861500	2.55020500
N	0.00000000	-1.94106200	1.25588500	N	-1.37253800	1.37253800	-1.25588500
N	1.94106200	0.00000000	1.25588500	N	1.37253800	-1.37253800	-1.25588500
N	-1.94106200	0.00000000	1.25588500	N	-1.37253800	-1.37253800	-1.25588500
N	2.36296100	2.36296100	1.52966800	N	1.37253800	1.37253800	-1.25588500
N	-2.36296100	-2.36296100	1.52966800	N	-3.34173100	0.00000000	-1.52966800
N	2.36296100	-2.36296100	1.52966800	N	3.34173100	0.00000000	-1.52966800
N	-2.36296100	2.36296100	1.52966800	N	0.00000000	-3.34173100	-1.52966800
C	1.10139800	2.72941900	1.47629800	N	0.00000000	3.34173100	-1.52966800
C	-1.10139800	2.72941900	1.47629800	C	-2.70879700	1.15118500	-1.47629800
C	2.72941900	-1.10139800	1.47629800	C	-1.15118500	2.70879700	-1.47629800
C	2.72941900	1.10139800	1.47629800	C	-1.15118500	-2.70879700	-1.47629800
C	-1.10139800	-2.72941900	1.47629800	C	-2.70879700	-1.15118500	-1.47629800
C	1.10139800	-2.72941900	1.47629800	C	2.70879700	-1.15118500	-1.47629800
C	-2.72941900	1.10139800	1.47629800	C	1.15118500	-2.70879700	-1.47629800
C	-2.72941900	-1.10139800	1.47629800	C	1.15118500	2.70879700	-1.47629800
C	0.69648500	4.09343600	1.76770600	C	2.70879700	1.15118500	-1.47629800
C	-0.69648500	4.09343600	1.76770600	C	-3.38698600	2.40200700	-1.76770600
C	4.09343600	-0.69648500	1.76770600	C	-2.40200700	3.38698600	-1.76770600
C	4.09343600	0.69648500	1.76770600	C	-2.40200700	-3.38698600	-1.76770600
C	-0.69648500	-4.09343600	1.76770600	C	-3.38698600	-2.40200700	-1.76770600
C	-4.09343600	0.69648500	1.76770600	C	3.38698600	-2.40200700	-1.76770600
C	-4.09343600	-0.69648500	1.76770600	C	2.40200700	-3.38698600	-1.76770600
C	1.42275700	5.24038600	2.05647800	C	2.40200700	3.38698600	-1.76770600
C	-1.42275700	5.24038600	2.05647800	C	3.38698600	2.40200700	-1.76770600
C	0.70058700	6.39691500	2.32680700	C	-4.71155300	2.69947100	-2.05647800
C	-0.70058700	6.39691500	2.32680700	C	-2.69947100	4.71155300	-2.05647800
C	5.24038600	-1.42275700	2.05647800	C	-5.01869200	4.02791200	-2.32680700
C	5.24038600	1.42275700	2.05647800	C	-4.02791200	5.01869200	-2.32680700
C	6.39691500	-0.70058700	2.32680700	C	-2.69947100	-4.71155300	-2.05647800
C	6.39691500	0.70058700	2.32680700	C	-4.71155300	-2.69947100	-2.05647800
C	-1.42275700	-5.24038600	2.05647800	C	-4.02791200	-5.01869200	-2.32680700
C	1.42275700	-5.24038600	2.05647800	C	-5.01869200	-4.02791200	-2.32680700
C	-0.70058700	-6.39691500	2.32680700	C	4.71155300	-2.69947100	-2.05647800
C	0.70058700	-6.39691500	2.32680700	C	2.69947100	-4.71155300	-2.05647800
C	-5.24038600	1.42275700	2.05647800	C	5.01869200	-4.02791200	-2.32680700
C	-5.24038600	-1.42275700	2.05647800	C	4.02791200	-5.01869200	-2.32680700
C	-6.39691500	0.70058700	2.32680700	C	2.69947100	4.71155300	-2.05647800
C	-6.39691500	-0.70058700	2.32680700	C	4.71155300	2.69947100	-2.05647800
H	2.50691500	5.22734000	2.06830000	C	4.02791200	5.01869200	-2.32680700
H	-2.50691500	5.22734000	2.06830000	C	5.01869200	4.02791200	-2.32680700
H	1.22861500	7.31838800	2.55020500	H	-5.46894400	1.92363000	-2.06830000
H	-1.22861500	7.31838800	2.55020500	H	-1.92363000	5.46894400	-2.06830000
H	5.22734000	-2.50691500	2.06830000	H	-6.04364400	4.30612000	-2.55020500
H	5.22734000	2.50691500	2.06830000	H	-4.30612000	6.04364400	-2.55020500
H	7.31838800	-1.22861500	2.55020500	H	-1.92363000	-5.46894400	-2.06830000
H	7.31838800	1.22861500	2.55020500	H	-5.46894400	-1.92363000	-2.06830000
H	-2.50691500	-5.22734000	2.06830000	H	-4.30612000	-6.04364400	-2.55020500
H	2.50691500	-5.22734000	2.06830000	H	-6.04364400	-4.30612000	-2.55020500
H	-1.22861500	-7.31838800	2.55020500	H	5.46894400	-1.92363000	-2.06830000
H	1.22861500	-7.31838800	2.55020500	H	1.92363000	-5.46894400	-2.06830000
H	-5.22734000	2.50691500	2.06830000	H	6.04364400	-4.30612000	-2.55020500
H	-5.22734000	-2.50691500	2.06830000	H	4.30612000	-6.04364400	-2.55020500
				H	1.92363000	5.46894400	-2.06830000
				H	5.46894400	1.92363000	-2.06830000
				H	4.30612000	6.04364400	-2.55020500
				H	6.04364400	4.30612000	-2.55020500

**Sc(Pc)<sub>2</sub> D<sub>2</sub> symmetry**

Sc	0.00000000	0.00000000	0.00000000	H	-6.28091100	3.71395900	2.90600000
N	0.75012500	1.73249500	1.35469600	H	-7.31641100	1.58484400	2.23347900
N	-0.75012500	-1.73249500	1.35469600	N	-0.75012500	1.73249500	-1.35469600
N	1.80947100	-0.76063700	1.09970100	N	0.75012500	-1.73249500	-1.35469600
N	-1.80947100	0.76063700	1.09970100	N	-1.80947100	-0.76063700	-1.09970100
N	3.13241800	1.28628900	1.32686100	N	1.80947100	0.76063700	-1.09970100
N	-3.13241800	-1.28628900	1.32686100	N	-3.13241800	1.28628900	-1.32686100
N	1.25857700	-2.93703800	1.92433100	N	3.13241800	-1.28628900	-1.32686100
N	-1.25857700	2.93703800	1.92433100	N	-1.25857700	-2.93703800	-1.92433100
C	2.09978500	2.01511100	1.55262400	N	1.25857700	2.93703800	-1.92433100
C	0.04432600	2.78285700	1.82996300	C	-2.09978500	2.01511100	-1.55262400
C	2.09985000	-1.94752400	1.59366100	C	-0.04432600	2.78285700	-1.82996300
C	3.02952300	-0.03533300	0.86105900	C	-2.09985000	-1.94752400	-1.59366100
C	-2.09978500	-2.01511100	1.55262400	C	-3.02952300	-0.03533300	-0.86105900
C	-0.04432600	-2.78285700	1.82996300	C	2.09978500	-2.01511100	-1.55262400
C	-2.09985000	1.94752400	1.59366100	C	0.04432600	-2.78285700	-1.82996300
C	-3.02952300	0.03533300	0.86105900	C	2.09985000	1.94752400	-1.59366100
C	2.23704600	3.36590000	2.13220200	C	3.02952300	0.03533300	-0.86105900
C	0.94720300	3.84143100	2.31355300	C	-2.23704600	3.36590000	-2.13220200
C	3.54516700	-2.09712200	1.79720500	C	-0.94720300	3.84143100	-2.31355300
C	4.13401800	-0.91252600	1.37661100	C	-3.54516700	-2.09712200	-1.79720500
C	-2.23704600	-3.36590000	2.13220200	C	-4.13401800	-0.91252600	-1.37661100
C	-0.94720300	-3.84143100	2.31355300	C	2.23704600	-3.36590000	-2.13220200
C	-3.54516700	2.09712200	1.79720500	C	0.94720300	-3.84143100	-2.31355300
C	-4.13401800	0.91252600	1.37661100	C	3.54516700	2.09712200	-1.79720500
C	3.34187600	4.11500600	2.49460200	C	4.13401800	0.91252600	-1.37661100
C	0.70248000	5.08713300	2.86519100	C	-3.34187600	4.11500600	-2.49460200
C	3.10767800	5.37507100	3.04178500	C	-0.70248000	5.08713300	-2.86519100
C	1.80819000	5.85413800	3.22487100	C	-3.10767800	5.37507100	-3.04178500
C	4.29121600	-3.12905600	2.34662900	C	-1.80819000	5.85413800	-3.22487100
C	5.48929500	-0.69243600	1.54390300	C	-4.29121600	-3.12905600	-2.34662900
C	5.66113700	-2.93159100	2.47867400	C	-5.48929500	-0.69243600	-1.54390300
C	6.24858000	-1.72457700	2.09249100	C	-5.66113700	-2.93159100	-2.47867400
C	-3.34187600	-4.11500600	2.49460200	C	-6.24858000	-1.72457700	-2.09249100
C	-0.70248000	-5.08713300	2.86519100	C	3.34187600	-4.11500600	-2.49460200
C	-3.10767800	-5.37507100	3.04178500	C	0.70248000	-5.08713300	-2.86519100
C	-1.80819000	-5.85413800	3.22487100	C	3.10767800	-5.37507100	-3.04178500
C	-4.29121600	3.12905600	2.34662900	C	1.80819000	-5.85413800	-3.22487100
C	-5.48929500	0.69243600	1.54390300	C	4.29121600	3.12905600	-2.34662900
C	-5.66113700	2.93159100	2.47867400	C	5.48929500	0.69243600	-1.54390300
C	-6.24858000	1.72457700	2.09249100	C	5.66113700	2.93159100	-2.47867400
H	4.34598400	3.73008800	2.35225000	C	6.24858000	1.72457700	-2.09249100
H	-0.31262700	5.44288000	3.00483300	H	-4.34598400	3.73008800	-2.35225000
H	3.94848300	5.99744500	3.33314800	H	0.31262700	5.44288000	-3.00483300
H	1.66121600	6.83976600	3.65609400	H	-3.94848300	5.99744500	-3.33314800
H	3.80883500	-4.04462500	2.67163300	H	-1.66121600	6.83976600	-3.65609400
H	5.93988700	0.25546600	1.27160700	H	-3.80883500	-4.04462500	-2.67163300
H	6.28091100	-3.71395900	2.90600000	H	-5.93988700	0.25546600	-1.27160700
H	7.31641100	-1.58484400	2.23347900	H	-6.28091100	-3.71395900	-2.90600000
H	-4.34598400	-3.73008800	2.35225000	H	-7.31641100	-1.58484400	-2.23347900
H	0.31262700	-5.44288000	3.00483300	H	4.34598400	-3.73008800	-2.35225000
H	-3.94848300	-5.99744500	3.33314800	H	-0.31262700	-5.44288000	-3.00483300
H	-1.66121600	-6.83976600	3.65609400	H	3.94848300	-5.99744500	-3.33314800
H	-3.80883500	4.04462500	2.67163300	H	1.66121600	-6.83976600	-3.65609400
H	-5.93988700	-0.25546600	1.27160700	H	3.80883500	4.04462500	-2.67163300
				H	5.93988700	-0.25546600	-1.27160700
				H	6.28091100	3.71395900	-2.90600000
				H	7.31641100	1.58484400	-2.23347900

**Sc(Pc)<sub>2</sub> D<sub>4d</sub> symmetry**

Sc	0.00000000	0.00000000	0.00000000	H	-7.33177400	1.22965500	2.57277400
N	0.00000000	1.95376100	1.27018800	H	-7.33177400	-1.22965500	2.57277400
N	0.00000000	-1.95376100	1.27018800	N	-1.38151800	1.38151800	-1.27018800
N	1.95376100	0.00000000	1.27018800	N	1.38151800	-1.38151800	-1.27018800
N	-1.95376100	0.00000000	1.27018800	N	-1.38151800	-1.38151800	-1.27018800
N	2.36100000	2.36100000	1.56167600	N	1.38151800	1.38151800	-1.27018800
N	-2.36100000	-2.36100000	1.56167600	N	-3.33895800	0.00000000	-1.56167600
N	2.36100000	-2.36100000	1.56167600	N	3.33895800	0.00000000	-1.56167600
N	-2.36100000	2.36100000	1.56167600	N	0.00000000	-3.33895800	-1.56167600
C	1.09594600	2.73038900	1.50287700	N	0.00000000	3.33895800	-1.56167600
C	-1.09594600	2.73038900	1.50287700	C	-2.70562700	1.15572600	-1.50287700
C	2.73038900	-1.09594600	1.50287700	C	-1.15572600	2.70562700	-1.50287700
C	2.73038900	1.09594600	1.50287700	C	-1.15572600	-2.70562700	-1.50287700
C	-1.09594600	-2.73038900	1.50287700	C	-2.70562700	-1.15572600	-1.50287700
C	1.09594600	-2.73038900	1.50287700	C	2.70562700	-1.15572600	-1.50287700
C	-2.73038900	1.09594600	1.50287700	C	1.15572600	-2.70562700	-1.50287700
C	-2.73038900	-1.09594600	1.50287700	C	1.15572600	2.70562700	-1.50287700
C	0.69667500	4.10186000	1.80172200	C	2.70562700	1.15572600	-1.50287700
C	-0.69667500	4.10186000	1.80172200	C	-3.39307700	2.40782900	-1.80172200
C	4.10186000	-0.69667500	1.80172200	C	-2.40782900	3.39307700	-1.80172200
C	4.10186000	0.69667500	1.80172200	C	-2.40782900	-3.39307700	-1.80172200
C	-0.69667500	-4.10186000	1.80172200	C	-3.39307700	-2.40782900	-1.80172200
C	-4.10186000	0.69667500	1.80172200	C	3.39307700	-2.40782900	-1.80172200
C	-4.10186000	-0.69667500	1.80172200	C	2.40782900	-3.39307700	-1.80172200
C	1.42064500	5.25015000	2.08667300	C	2.40782900	3.39307700	-1.80172200
C	-1.42064500	5.25015000	2.08667300	C	3.39307700	2.40782900	-1.80172200
C	0.70019100	6.40911500	2.35475000	C	-4.71696500	2.70786900	-2.08667300
C	-0.70019100	6.40911500	2.35475000	C	-2.70786900	4.71696500	-2.08667300
C	5.25015000	-1.42064500	2.08667300	C	-5.02703800	4.03681900	-2.35475000
C	5.25015000	1.42064500	2.08667300	C	-4.03681900	5.02703800	-2.35475000
C	6.40911500	-0.70019100	2.35475000	C	-2.70786900	-4.71696500	-2.08667300
C	6.40911500	0.70019100	2.35475000	C	-4.71696500	-2.70786900	-2.08667300
C	-1.42064500	-5.25015000	2.08667300	C	-4.03681900	-5.02703800	-2.35475000
C	1.42064500	-5.25015000	2.08667300	C	-5.02703800	-4.03681900	-2.35475000
C	-0.70019100	-6.40911500	2.35475000	C	4.71696500	-2.70786900	-2.08667300
C	0.70019100	-6.40911500	2.35475000	C	2.70786900	-4.71696500	-2.08667300
C	-5.25015000	1.42064500	2.08667300	C	5.02703800	-4.03681900	-2.35475000
C	-5.25015000	-1.42064500	2.08667300	C	4.03681900	-5.02703800	-2.35475000
C	-6.40911500	0.70019100	2.35475000	C	2.70786900	4.71696500	-2.08667300
C	-6.40911500	-0.70019100	2.35475000	C	4.71696500	2.70786900	-2.08667300
H	2.50522400	5.23591800	2.09393400	C	4.03681900	5.02703800	-2.35475000
H	-2.50522400	5.23591800	2.09393400	C	5.02703800	4.03681900	-2.35475000
H	1.22965500	7.33177400	2.57277400	H	-5.47381400	1.93089300	-2.09393400
H	-1.22965500	7.33177400	2.57277400	H	-1.93089300	5.47381400	-2.09393400
H	5.23591800	-2.50522400	2.09393400	H	-6.05384500	4.31485000	-2.57277400
H	5.23591800	2.50522400	2.09393400	H	-4.31485000	6.05384500	-2.57277400
H	7.33177400	-1.22965500	2.57277400	H	-1.93089300	-5.47381400	-2.09393400
H	7.33177400	1.22965500	2.57277400	H	-5.47381400	-1.93089300	-2.09393400
H	-2.50522400	-5.23591800	2.09393400	H	-4.31485000	-6.05384500	-2.57277400
H	2.50522400	-5.23591800	2.09393400	H	-6.05384500	-4.31485000	-2.57277400
H	-1.22965500	-7.33177400	2.57277400	H	5.47381400	-1.93089300	-2.09393400
H	1.22965500	-7.33177400	2.57277400	H	1.93089300	-5.47381400	-2.09393400
H	-5.23591800	2.50522400	2.09393400	H	6.05384500	-4.31485000	-2.57277400
H	-5.23591800	-2.50522400	2.09393400	H	4.31485000	-6.05384500	-2.57277400
				H	1.93089300	5.47381400	-2.09393400
				H	5.47381400	1.93089300	-2.09393400
				H	4.31485000	6.05384500	-2.57277400
				H	6.05384500	4.31485000	-2.57277400

**Sc(Pc)<sub>2</sub><sup>+</sup> D<sub>2</sub> symmetry**

Sc	0.00000000	0.00000000	0.00000000	H	-6.30473300	3.95852700	2.49113500
N	0.74832300	1.79808600	1.25242900	H	-7.24873500	1.69129900	2.49859100
N	-0.74832300	-1.79808600	1.25242900	N	-0.74832300	1.79808600	-1.25242900
N	1.79809800	-0.74827500	1.25243100	N	0.74832300	-1.79808600	-1.25242900
N	-1.79809800	0.74827500	1.25243100	N	-1.79809800	-0.74827500	-1.25243100
N	3.08761900	1.27236900	1.52565200	N	1.79809800	0.74827500	-1.25243100
N	-3.08761900	-1.27236900	1.52565200	N	-3.08761900	1.27236900	-1.52565200
N	1.27245300	-3.08762100	1.52501600	N	3.08761900	-1.27236900	-1.52565200
N	-1.27245300	3.08762100	1.52501600	N	-1.27245300	-3.08762100	-1.52501600
C	2.06057800	2.09880400	1.46915000	N	1.27245300	3.08762100	-1.52501600
C	0.03800500	2.94098100	1.47033200	C	-2.06057800	2.09880400	-1.46915000
C	2.09893900	-2.06064400	1.46825400	C	-0.03800500	2.94098100	-1.47033200
C	2.94107300	-0.03804900	1.47017900	C	-2.09893900	-2.06064400	-1.46825400
C	-2.06057800	-2.09880400	1.46915000	C	-2.94107300	-0.03804900	-1.47017900
C	-0.03800500	-2.94098100	1.47033200	C	2.06057800	-2.09880400	-1.46915000
C	-2.09893900	2.06064400	1.46825400	C	0.03800500	-2.94098100	-1.47033200
C	-2.94107300	0.03804900	1.47017900	C	2.09893900	2.06064400	-1.46825400
C	2.22159600	3.52393500	1.75493000	C	2.94107300	0.03804900	-1.47017900
C	0.93612900	4.05907800	1.75735800	C	-2.22159600	3.52393500	-1.75493000
C	3.52425100	-2.22178700	1.75311300	C	-0.93612900	4.05907800	-1.75735800
C	4.05937500	-0.93630000	1.75590400	C	-3.52425100	-2.22178700	-1.75311300
C	-2.22159600	-3.52393500	1.75493000	C	-4.05937500	-0.93630000	-1.75590400
C	-0.93612900	-4.05907800	1.75735800	C	2.22159600	-3.52393500	-1.75493000
C	-3.52425100	2.22178700	1.75311300	C	0.93612900	-4.05907800	-1.75735800
C	-4.05937500	0.93630000	1.75590400	C	3.52425100	2.22178700	-1.75311300
C	3.33307900	4.30303100	2.02641900	C	4.05937500	0.93630000	-1.75590400
C	0.70822200	5.39654800	2.03291800	C	-3.33307900	4.30303100	-2.02641900
C	3.11388300	5.65515500	2.28486200	C	-0.70822200	5.39654800	-2.03291800
C	1.82390600	6.19228600	2.28862700	C	-3.11388300	5.65515500	-2.28486200
C	4.30352400	-3.33337700	2.02362000	C	-1.82390600	6.19228600	-2.28862700
C	5.39700700	-0.70851100	2.03079000	C	4.30352400	-3.33337700	-2.02362000
C	5.65580500	-3.11429200	2.28135100	C	5.39700700	-0.70851100	-2.03079000
C	6.19292300	-1.82431200	2.28544100	C	5.65580500	-3.11429200	-2.28135100
C	-3.33307900	-4.30303100	2.02641900	C	6.19292300	-1.82431200	-2.28544100
C	-0.70822200	-5.39654800	2.03291800	H	-4.32901300	3.87413500	-2.03559200
C	-3.11388300	-5.65515500	2.28486200	H	0.29742100	5.80211700	-2.04764200
C	-1.82390600	-6.19228600	2.28862700	H	-3.95802000	6.30394600	-2.49545900
C	-4.30352400	3.33337700	2.02362000	H	-1.69080400	7.24797100	-2.50234500
C	-5.39700700	0.70851100	2.03079000	H	-3.87464700	-4.32932100	-2.03256300
C	-5.65580500	3.11429200	2.28135100	H	-5.80256200	0.29713500	-2.04579300
C	-6.19292300	1.82431200	2.28544100	H	-6.30473300	-3.95852700	-2.49113500
H	4.32901300	3.87413500	2.03559200	H	-7.24873500	-1.69129900	-2.49859100
H	-0.29742100	5.80211700	2.04764200	H	4.32901300	-3.87413500	-2.03559200
H	3.95802000	6.30394600	2.49545900	H	-0.29742100	-5.80211700	-2.04764200
H	1.69080400	7.24797100	2.50234500	H	3.95802000	-6.30394600	-2.49545900
H	3.87464700	-4.32932100	2.03256300	H	1.69080400	-7.24797100	-2.50234500
H	5.80256200	0.29713500	2.04579300	H	3.87464700	4.32932100	-2.03256300
H	6.30473300	-3.95852700	2.49113500	H	5.80256200	-0.29713500	-2.04579300
H	7.24873500	-1.69129900	2.49859100	H	6.30473300	3.95852700	-2.49113500
H	-4.32901300	-3.87413500	2.03559200	H	-3.87464700	4.32932100	-2.03256300
H	0.29742100	-5.80211700	2.04764200	H	5.80256200	-0.29713500	-2.04579300
H	-3.95802000	-6.30394600	2.49545900	H	7.24873500	1.69129900	-2.49859100
H	-1.69080400	-7.24797100	2.50234500				
H	-3.87464700	4.32932100	2.03256300				
H	-5.80256200	-0.29713500	2.04579300				

**Sc(Pc)<sub>2</sub><sup>+</sup> D<sub>4d</sub> symmetry**

Sc	0.00000000	0.00000000	0.00000000	H	-7.33666100	1.22784700	2.51770300
N	0.00000000	1.94746400	1.25246000	H	-7.33666100	-1.22784700	2.51770300
N	0.00000000	-1.94746400	1.25246000	N	-1.37706500	1.37706500	-1.25246000
N	1.94746400	0.00000000	1.25246000	N	1.37706500	-1.37706500	-1.25246000
N	-1.94746400	0.00000000	1.25246000	N	-1.37706500	-1.37706500	-1.25246000
N	2.36148200	2.36148200	1.52565000	N	1.37706500	1.37706500	-1.25246000
N	-2.36148200	-2.36148200	1.52565000	N	-3.33964000	0.00000000	-1.52565000
N	2.36148200	-2.36148200	1.52565000	N	3.33964000	0.00000000	-1.52565000
N	-2.36148200	2.36148200	1.52565000	N	0.00000000	-3.33964000	-1.52565000
C	1.09542700	2.72950800	1.47025000	N	0.00000000	3.33964000	-1.52565000
C	-1.09542700	2.72950800	1.47025000	C	-2.70463700	1.15547000	-1.47025000
C	2.72950800	-1.09542700	1.47025000	C	-1.15547000	2.70463700	-1.47025000
C	2.72950800	1.09542700	1.47025000	C	-1.15547000	-2.70463700	-1.47025000
C	-1.09542700	-2.72950800	1.47025000	C	-2.70463700	-1.15547000	-1.47025000
C	1.09542700	-2.72950800	1.47025000	C	2.70463700	-1.15547000	-1.47025000
C	-2.72950800	1.09542700	1.47025000	C	1.15547000	-2.70463700	-1.47025000
C	-2.72950800	-1.09542700	1.47025000	C	1.15547000	2.70463700	-1.47025000
C	0.69616200	4.10642200	1.75884100	C	2.70463700	1.15547000	-1.47025000
C	-0.69616200	4.10642200	1.75884100	C	-3.39593900	2.41141800	-1.75884100
C	4.10642200	-0.69616200	1.75884100	C	-2.41141800	3.39593900	-1.75884100
C	4.10642200	0.69616200	1.75884100	C	-2.41141800	-3.39593900	-1.75884100
C	-0.69616200	-4.10642200	1.75884100	C	-3.39593900	-2.41141800	-1.75884100
C	0.69616200	-4.10642200	1.75884100	C	3.39593900	-2.41141800	-1.75884100
C	-4.10642200	0.69616200	1.75884100	C	2.41141800	-3.39593900	-1.75884100
C	-4.10642200	-0.69616200	1.75884100	C	2.41141800	3.39593900	-1.75884100
C	1.42183200	5.25184900	2.03800100	C	3.39593900	2.41141800	-1.75884100
C	-1.42183200	5.25184900	2.03800100	C	-4.71900500	2.70823100	-2.03800100
C	0.69869400	6.41424600	2.30084600	C	-2.70823100	4.71900500	-2.03800100
C	-0.69869400	6.41424600	2.30084600	C	-5.02960800	4.04150500	-2.30084600
C	5.25184900	-1.42183200	2.03800100	C	-4.04150500	5.02960800	-2.30084600
C	5.25184900	1.42183200	2.03800100	C	-2.70823100	-4.71900500	-2.03800100
C	6.41424600	-0.69869400	2.30084600	C	-4.71900500	-2.70823100	-2.03800100
C	6.41424600	0.69869400	2.30084600	C	-4.04150500	-5.02960800	-2.30084600
C	-1.42183200	-5.25184900	2.03800100	C	-5.02960800	-4.04150500	-2.30084600
C	1.42183200	-5.25184900	2.03800100	C	4.71900500	-2.70823100	-2.03800100
C	-0.69869400	-6.41424600	2.30084600	C	2.70823100	-4.71900500	-2.03800100
C	0.69869400	-6.41424600	2.30084600	C	5.02960800	-4.04150500	-2.30084600
C	-5.25184900	1.42183200	2.03800100	C	4.04150500	-5.02960800	-2.30084600
C	-5.25184900	-1.42183200	2.03800100	C	2.70823100	4.71900500	-2.03800100
C	-6.41424600	0.69869400	2.30084600	C	4.71900500	2.70823100	-2.03800100
C	-6.41424600	-0.69869400	2.30084600	C	4.04150500	5.02960800	-2.30084600
H	2.50609100	5.23906000	2.05059200	C	5.02960800	4.04150500	-2.30084600
H	-2.50609100	5.23906000	2.05059200	H	-5.47664900	1.93250100	-2.05059200
H	1.22784700	7.33666100	2.51770300	H	-1.93250100	5.47664900	-2.05059200
H	-1.22784700	7.33666100	2.51770300	H	-6.05602200	4.31958400	-2.51770300
H	5.23906000	-2.50609100	2.05059200	H	-4.31958400	6.05602200	-2.51770300
H	5.23906000	2.50609100	2.05059200	H	-1.93250100	-5.47664900	-2.05059200
H	7.33666100	-1.22784700	2.51770300	H	-5.47664900	-1.93250100	-2.05059200
H	7.33666100	1.22784700	2.51770300	H	-4.31958400	-6.05602200	-2.51770300
H	-2.50609100	-5.23906000	2.05059200	H	-6.05602200	-4.31958400	-2.51770300
H	2.50609100	-5.23906000	2.05059200	H	5.47664900	-1.93250100	-2.05059200
H	-1.22784700	-7.33666100	2.51770300	H	1.93250100	-5.47664900	-2.05059200
H	1.22784700	-7.33666100	2.51770300	H	6.05602200	-4.31958400	-2.51770300
H	-5.23906000	2.50609100	2.05059200	H	4.31958400	-6.05602200	-2.51770300
H	-5.23906000	-2.50609100	2.05059200	H	1.93250100	5.47664900	-2.05059200
				H	5.47664900	1.93250100	-2.05059200
				H	4.31958400	6.05602200	-2.51770300
				H	6.05602200	4.31958400	-2.51770300