Additive decomposition of the physical components of the magnetic coupling from broken symmetry density functional theory calculations: Supplementary Informations

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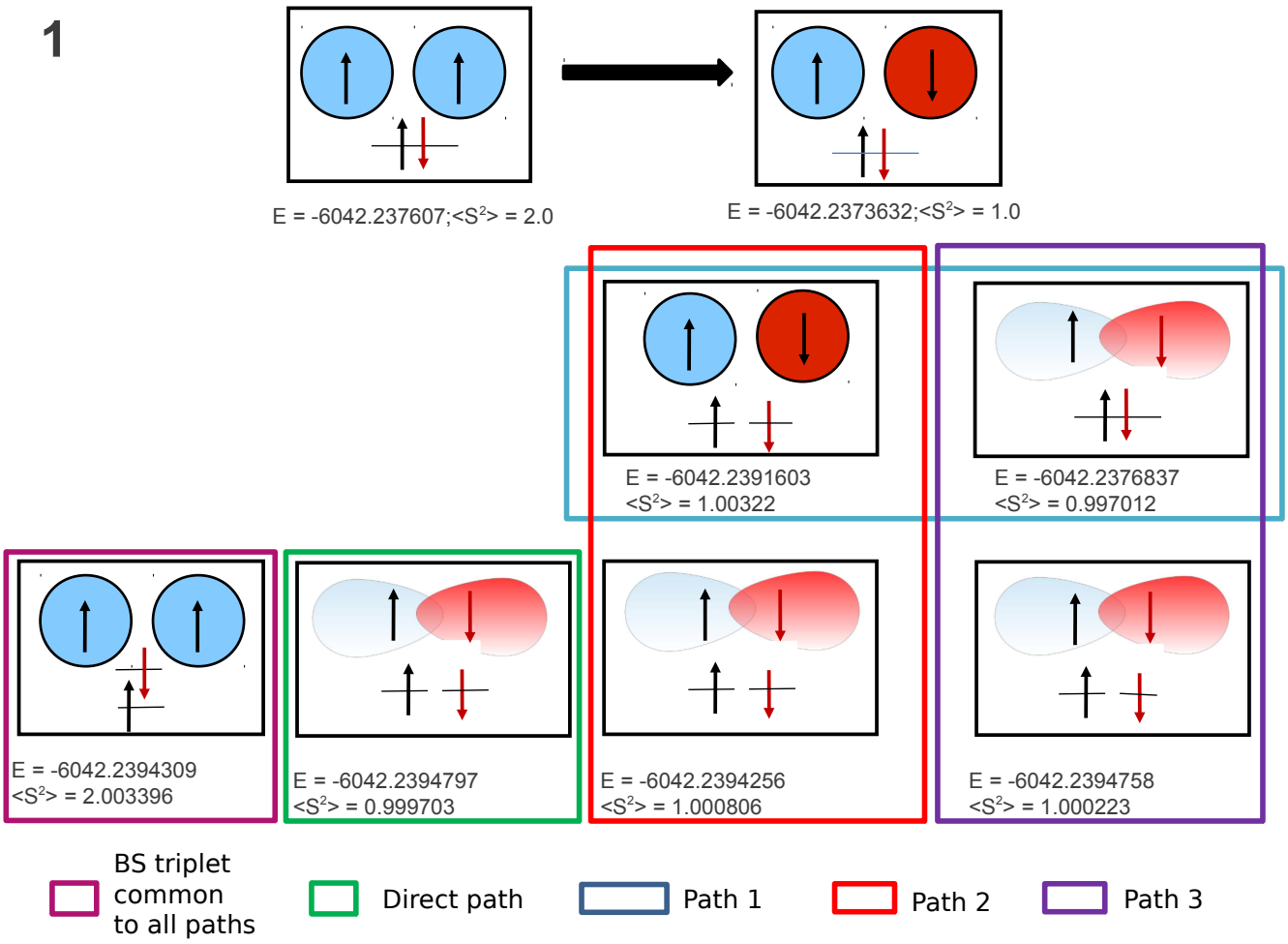
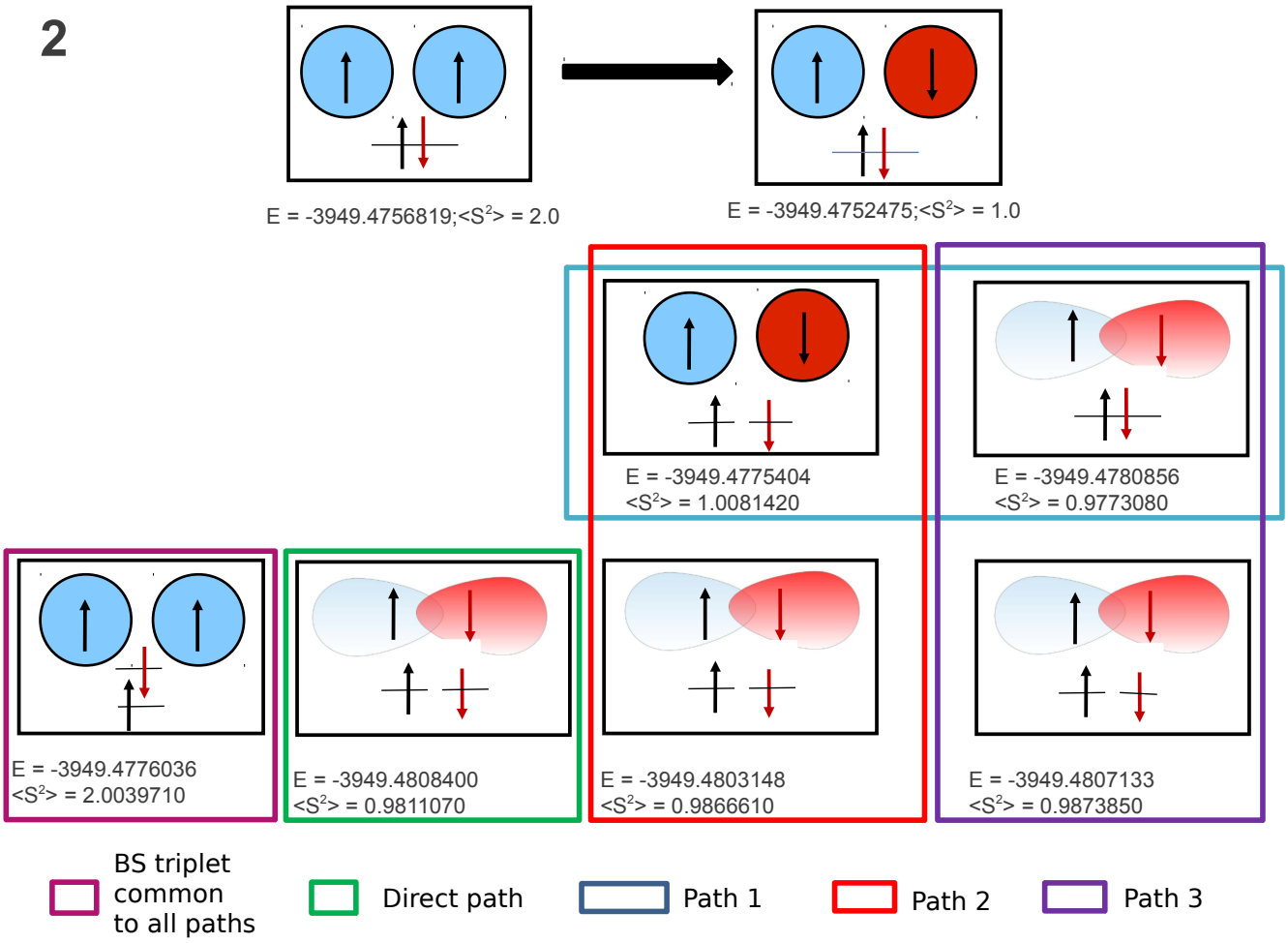
1 Energies and $\langle \mathscr{S}^2 \rangle$ (in a.u.)

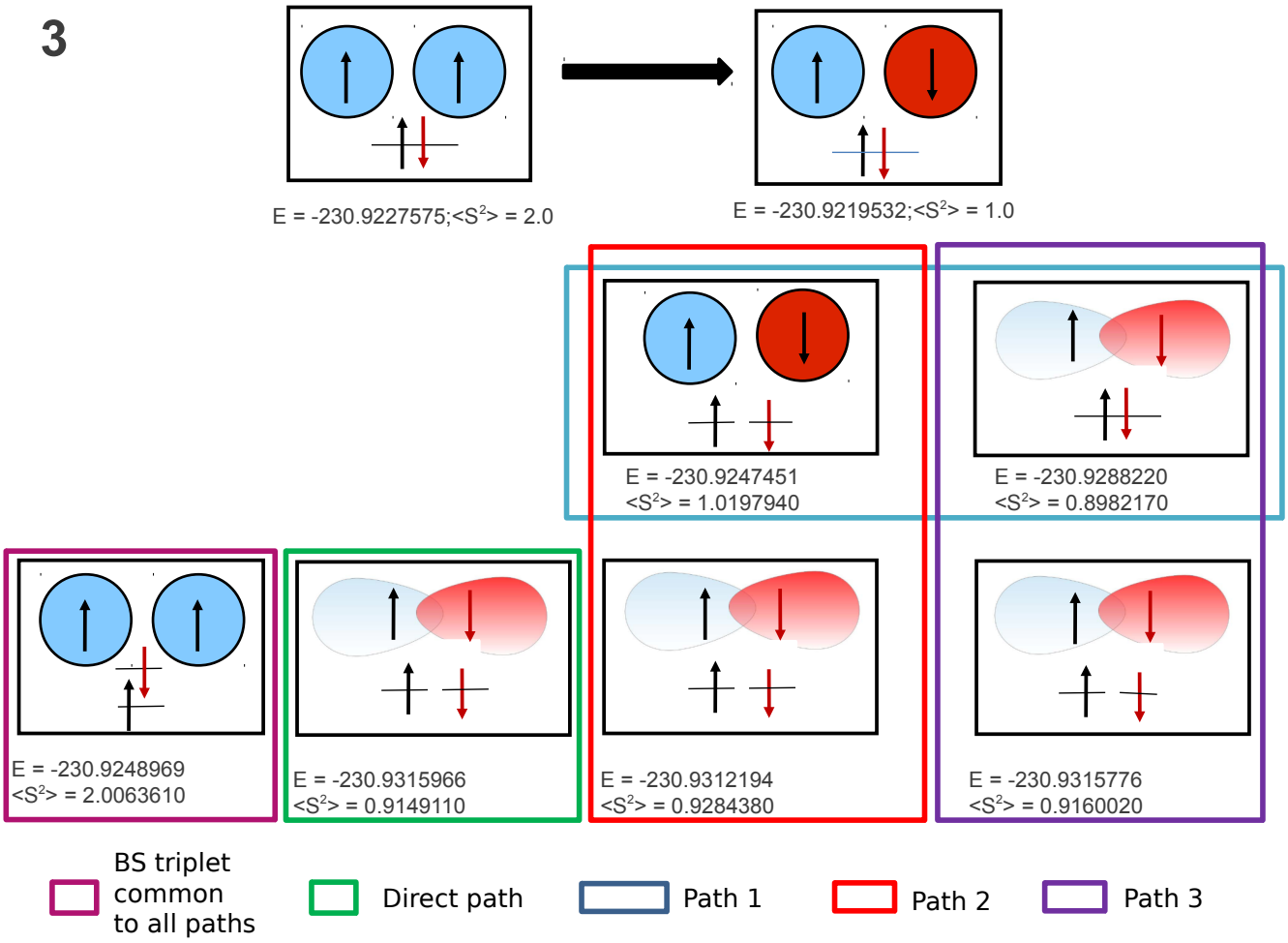
Cu_2-chlorine **1**



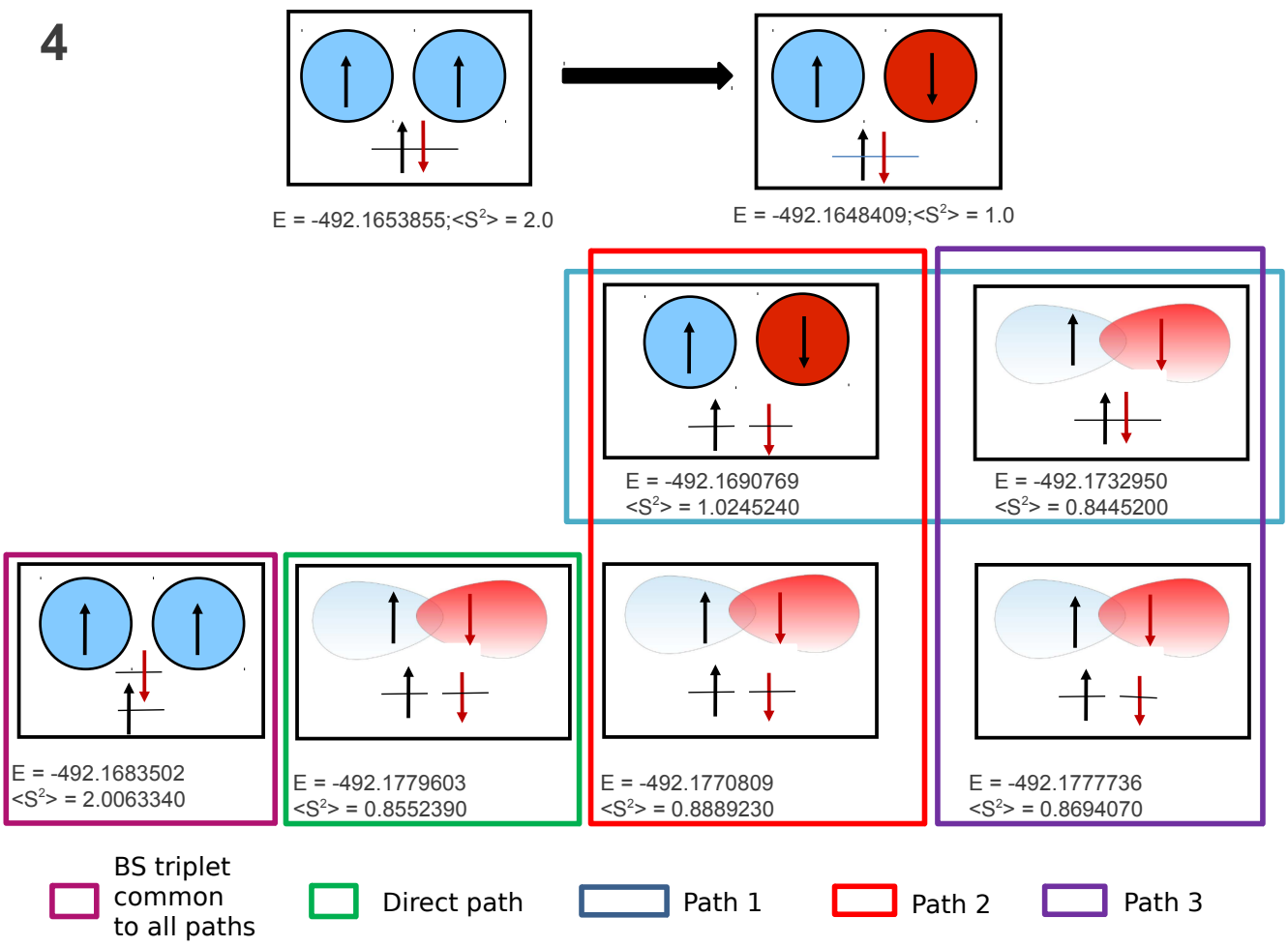
Cu_2-azido **2**


2
E = -3949.4756819;<S²> = 2.0
E = -3949.4752475;<S²> = 1.0
E = -3949.4775404
<S²> = 1.0081420
E = -3949.4780856
<S²> = 0.9773080
E = -3949.4776036
<S²> = 2.0039710
E = -3949.4808400
<S²> = 0.9811070
E = -3949.4803148
<S²> = 0.9866610
E = -3949.4807133
<S²> = 0.9873850
BS triplet common to all paths
Direct path
Path 1
Path 2
Path 3

p-benzyne **3**


3
E = -230.9227575;<S²> = 2.0
E = -230.9219532;<S²> = 1.0
E = -230.9247451
<S²> = 1.0197940
E = -230.9288220
<S²> = 0.8982170
E = -230.9248969
<S²> = 2.0063610
E = -230.9315966
<S²> = 0.9149110
E = -230.9312194
<S²> = 0.9284380
E = -230.9315776
<S²> = 0.9160020
BS triplet common to all paths
Direct path
Path 1
Path 2
Path 3

bis-nitroxide **4**



2 Geometries

Cu_2-chlorine **1**

Cu	0.000000	0.000000	1.719999
Cu	0.000000	0.000000	-1.719999
CL	1.552043	0.000000	0.000000
CL	-1.552043	0.000000	0.000000
CL	1.642058	0.000000	3.272817
CL	-1.642058	0.000000	3.272817
CL	1.642058	0.000000	-3.272817
CL	-1.642058	0.000000	-3.272817

Cu_2-azido **2**

CU	0.000000	0.000000	2.596298
CU	0.000000	0.000000	-2.596298
N	1.403778	0.000000	1.157614
N	-1.403778	0.000000	1.157614
N	1.403778	0.000000	-1.157614
N	-1.403778	0.000000	-1.157614
N	1.403754	0.000000	0.000000
N	-1.403754	0.000000	0.000000
N	1.433693	0.000000	4.064581
N	-1.433693	0.000000	4.064581
N	1.433693	0.000000	-4.064581
N	-1.433693	0.000000	-4.064581
N	0.000000	-2.243659	2.539065
N	0.000000	2.243659	-2.539065
H	1.990565	0.709744	3.993129

H	−1.990565	0.709744	3.993129
H	1.990565	−0.709744	−3.993129
H	−1.990565	−0.709744	−3.993129
H	1.014016	0.000000	4.916817
H	−1.014016	0.000000	4.916817
H	1.014016	0.000000	−4.916817
H	−1.014016	0.000000	−4.916817
H	1.959943	−0.841008	3.963249
H	−1.959943	−0.841008	3.963249
H	1.959943	0.841008	−3.963249
H	−1.959943	0.841008	−3.963249
H	0.000000	−2.583062	3.426368
H	0.000000	2.583062	−3.426368
H	0.775671	−2.548803	2.083302
H	−0.775671	−2.548803	2.083302
H	0.775671	2.548803	−2.083302
H	−0.775671	2.548803	−2.083302

p-benzyne **3**

C	1.205978	−0.716823	0.000000
C	1.206017	0.716844	0.000000
C	0.000000	1.352848	0.000000
C	−1.205996	0.716836	0.000000
C	−1.206009	−0.716832	0.000000
C	0.000003	−1.352885	0.000000
H	−2.161047	1.228522	0.000000
H	−2.161132	−1.228372	0.000000
H	2.161071	−1.228431	0.000000

H	2.161153	1.228351	0.000000

bis-nitroxide **4**

O	3.62565	0.42019	0.00000
O	-3.62565	-0.42019	0.00000
N	2.74337	-0.47994	0.00000
N	-2.74337	0.47994	0.00000
C	0.47300	-1.31433	0.00000
C	-0.47300	1.31433	0.00000
C	1.35538	-0.23125	0.00000
C	-1.35538	0.23125	0.00000
C	0.89873	1.08771	0.00000
C	-0.89873	-1.08771	0.00000
H	0.85333	-2.33904	0.00000
H	-0.85333	2.33904	0.00000
H	1.61982	1.90569	0.00000
H	-1.61982	-1.90569	0.00000
H	3.05114	-1.47155	0.00000
H	-3.05114	1.47155	0.00000