The Essential Role of Symmetry in Understanding ^{3}He Chemical Shifts in Endohedral Helium Fullerenes

Supporting Information

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Table S1: Energies of selected frontier orbitals (eV).

Molecule	*Orbital*	*Energy (eV)*	*Molecule*	*Orbital*	*Energy (eV)*
He@C_{60}	$7t_{1u}$	-9.054	He@C_{70}	$19e_1''$	-7.416
	$6h_u$	-7.525		$14a_2''$	-7.361
	$10h_g$	-3.268		$20e_1''$	-3.346
				$6a_1''$	-2.7
He@C_{60}^{6-}	$7t_{1u}$	10.345		$18a_1'$	-2.273
	$6h_u$	12.803			
	$10h_g$	15.33	He@C_{70}^{6-}	$19e_1''$	9.175
He@C_{60}^{10+}				$14a_2''$	9.314
	$7t_{1u}$	-39.737		$6a_1''$	11.533
	$6h_u$	-36.969		$20e_1''$	13.898
	$10h_g$	-34.539		$18a_1'$	15.474

Table S2: The diamagnetic and paramagnetic contributions to the ^{3}He nuclear shielding constant (σ) and calculated, as well as experimental δ(^{3}He) in He@C_n (n = 60, 76, 78, 84) series of endohedral He fullerenes.

Molecule	$\sigma_{\mathrm{He}}^{d+s1}$	σ_K^d	σ_K^p	δ(^{3}He)$_{calc}$	**δ(^{3}He)$_{exp}$**
He@C_{60}^{12-}	37.1	**300.9**	-263.8	**22.9**	**-**
^{3}He@D_2(1)-C_{76}	79.9	**297.1**	-217.2	**-19.9**	-18.8
^{3}He@D_2(1)-C_{76}^{6-}	83.7	**312.0**	-228.3	**-23.7**	-20.6
^{3}He@C_{2v}(3)-C_{78}	78.6	**301.9**	-223.2	**-18.7**	-17.6
^{3}He@C_{2v}(3)-C_{78}^{6-}	79.2	**316.2**	-237.0	**-19.2**	-13.5*
^{3}He@C_{2v}(2)-C_{78}	78.0	**300.2**	-222.2	**-18.0**	-16.9
^{3}He@C_{2v}(2)-C_{78}^{4-}	72.9	**310.9**	-237.9	**-13.0**	-10.0
^{3}He@D_2(22)C_{84}	69.1	**307.9**	-238.7	**-9.2**	-7.5
^{3}He@D_2(22)C_{84}^{6-}	86.9	**322.4**	-235.5	**-26.9**	-24.4
^{3}He@D_{2d}(4)C_{84}	86.3	**308.4**	-222.1	**-26.3**	-22.8
^{3}He@D_{2d}(4)C_{84}^{6-}	80.7	**322.4**	-241.8	**-20.7**	-22.1

*Probably a ^{3}He@C_{2v}(3)-C_{78}^{4-} (tetra-anion)

Geometry coordinates:

^{3}He@I_h-C_{60}
61

He	0.000000	0.000000	0.000000
C	-1.237374	0.000000	3.332981
C	-0.382370	-1.176812	3.332981
C	1.001056	-0.727310	3.332981
C	1.001056	0.727310	3.332981
C	-0.382370	1.176812	3.332981
C	2.346451	-2.603801	0.595182
C	3.201455	-1.426989	0.595182
C	2.965138	-0.699679	1.832556
C	1.964082	-1.426989	2.597295
C	1.581712	-2.603801	1.832556
C	3.201455	1.426989	0.595182
C	2.346451	2.603801	0.595182
C	1.581712	2.603801	1.832556

C	1.964082	1.426989	2.597295
C	2.965138	0.699679	1.832556
C	-0.367843	3.485729	0.595182
C	-1.751269	3.036226	0.595182
C	-1.987586	2.308916	1.832556
C	-0.750212	2.308916	2.597295
C	0.250844	3.036226	1.832556
C	-3.428795	0.727310	0.595182
C	-3.428795	-0.727310	0.595182
C	-2.810108	-1.176812	1.832556
C	-2.427738	0.000000	2.597295
C	-2.810108	1.176812	1.832556
C	-1.751269	-3.036226	0.595182
C	-0.367843	-3.485729	0.595182
C	0.250844	-3.036226	1.832556
C	-0.750212	-2.308916	2.597295
C	-1.987586	-2.308916	1.832556
C	-0.250844	-3.036226	-1.832556
C	0.750212	-2.308916	-2.597295
C	1.987586	-2.308916	-1.832556
C	1.751269	-3.036226	-0.595182
C	0.367843	-3.485729	-0.595182
C	2.810108	-1.176812	-1.832556
C	2.427738	0.000000	-2.597295
C	2.810108	1.176812	-1.832556
C	3.428795	0.727310	-0.595182
C	3.428795	-0.727310	-0.595182
C	1.987586	2.308916	-1.832556
C	0.750212	2.308916	-2.597295
C	-0.250844	3.036226	-1.832556
C	0.367843	3.485729	-0.595182
C	1.751269	3.036226	-0.595182
C	-1.581712	2.603801	-1.832556
C	-1.964082	1.426989	-2.597295
C	-2.965138	0.699679	-1.832556
C	-3.201455	1.426989	-0.595182
C	-2.346451	2.603801	-0.595182
C	-2.965138	-0.699679	-1.832556
C	-1.964082	-1.426989	-2.597295
C	-1.581712	-2.603801	-1.832556
C	-2.346451	-2.603801	-0.595182
C	-3.201455	-1.426989	-0.595182
C	-1.001056	-0.727310	-3.332981
C	-1.001056	0.727310	-3.332981
C	0.382370	1.176812	-3.332981
C	1.237374	0.000000	-3.332981
C	0.382370	-1.176812	-3.332981

$^{3}He@I_h\text{-}C_{60}^{6-}$

61

C	-1.237816	0.000000	3.368034
C	-0.382506	-1.177233	3.368034
C	1.001414	-0.727570	3.368034
C	1.001414	0.727570	3.368034
C	-0.382506	1.177233	3.368034
C	2.371793	-2.622534	0.610539
C	3.227102	-1.445301	0.610539
C	2.990700	-0.717731	1.848354
C	1.989286	-1.445301	2.613367
C	1.606780	-2.622534	1.848354
C	3.227102	1.445301	0.610539
C	2.371793	2.622534	0.610539
C	1.606780	2.622534	1.848354
C	1.989286	1.445301	2.613367
C	2.990700	0.717731	1.848354
C	-0.377334	3.515779	0.610539
C	-1.761254	3.066116	0.610539
C	-1.997655	2.338546	1.848354
C	-0.759840	2.338546	2.613367
C	0.241574	3.066116	1.848354
C	-3.460307	0.727570	0.610539
C	-3.460307	-0.727570	0.610539
C	-2.841399	-1.177233	1.848354
C	-2.458893	0.000000	2.613367
C	-2.841399	1.177233	1.848354
C	-1.761254	-3.066116	0.610539
C	-0.377334	-3.515779	0.610539
C	0.241574	-3.066116	1.848354
C	-0.759840	-2.338546	2.613367
C	-1.997655	-2.338546	1.848354
C	-0.241574	-3.066116	-1.848354
C	0.759840	-2.338546	-2.613367
C	1.997655	-2.338546	-1.848354
C	1.761254	-3.066116	-0.610539
C	0.377334	-3.515779	-0.610539
C	2.841399	-1.177233	-1.848354
C	2.458893	0.000000	-2.613367
C	2.841399	1.177233	-1.848354
C	3.460307	0.727570	-0.610539
C	3.460307	-0.727570	-0.610539
C	1.997655	2.338546	-1.848354
C	0.759840	2.338546	-2.613367
C	-0.241574	3.066116	-1.848354
C	0.377334	3.515779	-0.610539
C	1.761254	3.066116	-0.610539
C	-1.606780	2.622534	-1.848354
C	-1.989286	1.445301	-2.613367

C	-2.990700	0.717731	-1.848354
C	-3.227102	1.445301	-0.610539
C	-2.371793	2.622534	-0.610539
C	-2.990700	-0.717731	-1.848354
C	-1.989286	-1.445301	-2.613367
C	-1.606780	-2.622534	-1.848354
C	-2.371793	-2.622534	-0.610539
C	-3.227102	-1.445301	-0.610539
C	-1.001414	-0.727570	-3.368034
C	-1.001414	0.727570	-3.368034
C	0.382506	1.177233	-3.368034
C	1.237816	0.000000	-3.368034
C	0.382506	-1.177233	-3.368034
He	0.000000	0.000000	0.000000

$^{3}He@I_h$-C_{60}^{10+}

61

He	0.000000	0.000000	0.000000
C	-1.244558	0.000000	3.376236
C	-0.384590	-1.183645	3.376236
C	1.006869	-0.731533	3.376236
C	1.006869	0.731533	3.376236
C	-0.384590	1.183645	3.376236
C	2.377372	-2.631486	0.609328
C	3.237341	-1.447841	0.609328
C	2.999651	-0.716308	1.853886
C	1.992782	-1.447841	2.623066
C	1.608193	-2.631486	1.853886
C	3.237341	1.447841	0.609328
C	2.377372	2.631486	0.609328
C	1.608193	2.631486	1.853886
C	1.992782	1.447841	2.623066
C	2.999651	0.716308	1.853886
C	-0.376585	3.526301	0.609328
C	-1.768044	3.074189	0.609328
C	-2.005733	2.342656	1.853886
C	-0.761175	2.342656	2.623066
C	0.245694	3.074189	1.853886
C	-3.470083	0.731533	0.609328
C	-3.470083	-0.731533	0.609328
C	-2.847804	-1.183645	1.853886
C	-2.463214	0.000000	2.623066
C	-2.847804	1.183645	1.853886
C	-1.768044	-3.074189	0.609328
C	-0.376585	-3.526301	0.609328
C	0.245694	-3.074189	1.853886
C	-0.761175	-2.342656	2.623066
C	-2.005733	-2.342656	1.853886

C -0.245694 -3.074189 -1.853886
C 0.761175 -2.342656 -2.623066
C 2.005733 -2.342656 -1.853886
C 1.768044 -3.074189 -0.609328
C 0.376585 -3.526301 -0.609328
C 2.847804 -1.183645 -1.853886
C 2.463214 0.000000 -2.623066
C 2.847804 1.183645 -1.853886
C 3.470083 0.731533 -0.609328
C 3.470083 -0.731533 -0.609328
C 2.005733 2.342656 -1.853886
C 0.761175 2.342656 -2.623066
C -0.245694 3.074189 -1.853886
C 0.376585 3.526301 -0.609328
C 1.768044 3.074189 -0.609328
C -1.608193 2.631486 -1.853886
C -1.992782 1.447841 -2.623066
C -2.999651 0.716308 -1.853886
C -3.237341 1.447841 -0.609328
C -2.377372 2.631486 -0.609328
C -2.999651 -0.716308 -1.853886
C -1.992782 -1.447841 -2.623066
C -1.608193 -2.631486 -1.853886
C -2.377372 -2.631486 -0.609328
C -3.237341 -1.447841 -0.609328
C -1.006869 -0.731533 -3.376236
C -1.006869 0.731533 -3.376236
C 0.384590 1.183645 -3.376236
C 1.244558 0.000000 -3.376236
C 0.384590 -1.183645 -3.376236

^{3}He@D_{5h}(1)-C_{70}
71

C 0.747852 -2.301651 -3.222106
C 1.970779 -2.293643 -2.443798
C 0.381954 -1.175534 -3.970039
C 2.790388 -1.165547 -2.443798
C 3.400451 -0.720101 -1.208698
C 3.258042 -1.458042 0.000000
C 3.400451 -0.720101 1.208698
C -1.957902 -1.422499 -3.222106
C -1.572380 -2.583097 -2.443798
C -0.999969 -0.726520 -3.970039
C -0.246224 -3.013991 -2.443798
C 0.365941 -3.456544 -1.208698
C -0.379890 -3.549142 0.000000
C 0.365941 -3.456544 1.208698

C	2.393470	-2.648022	0.000000
C	1.735654	-3.011497	-1.208698
C	1.735654	-3.011497	1.208698
C	-1.957902	1.422499	-3.222106
C	-2.942563	0.697201	-2.443798
C	-0.999969	0.726520	-3.970039
C	-2.942563	-0.697201	-2.443798
C	-3.174287	-1.416161	-1.208698
C	-3.492827	-0.735448	0.000000
C	-3.174287	-1.416161	1.208698
C	-1.778796	-3.094609	0.000000
C	-2.327758	-2.581309	-1.208698
C	-2.327758	-2.581309	1.208698
C	0.747852	2.301651	-3.222106
C	-0.246224	3.013991	-2.443798
C	0.381954	1.175534	-3.970039
C	-1.572380	2.583097	-2.443798
C	-2.327758	2.581309	-1.208698
C	-1.778796	3.094609	0.000000
C	-2.327758	2.581309	1.208698
C	-3.492827	0.735448	0.000000
C	-3.174287	1.416161	-1.208698
C	-3.174287	1.416161	1.208698
C	2.420099	0.000000	-3.222106
C	2.790388	1.165547	-2.443798
C	1.236029	0.000000	-3.970039
C	1.970779	2.293643	-2.443798
C	1.735654	3.011497	-1.208698
C	2.393470	2.648022	0.000000
C	1.735654	3.011497	1.208698
C	-0.379890	3.549142	0.000000
C	0.365941	3.456544	-1.208698
C	0.365941	3.456544	1.208698
C	3.258042	1.458042	0.000000
C	3.400451	0.720101	-1.208698
C	3.400451	0.720101	1.208698
C	0.747852	2.301651	3.222106
C	1.970779	2.293643	2.443798
C	2.790388	1.165547	2.443798
C	0.381954	1.175534	3.970039
C	-1.957902	1.422499	3.222106
C	-1.572380	2.583097	2.443798
C	-0.246224	3.013991	2.443798
C	-0.999969	0.726520	3.970039
C	-1.957902	-1.422499	3.222106
C	-2.942563	-0.697201	2.443798
C	-2.942563	0.697201	2.443798
C	-0.999969	-0.726520	3.970039
C	0.747852	-2.301651	3.222106
C	-0.246224	-3.013991	2.443798
C	-1.572380	-2.583097	2.443798

C 0.381954 -1.175534 3.970039
C 2.420099 0.000000 3.222106
C 2.790388 -1.165547 2.443798
C 1.970779 -2.293643 2.443798
C 1.236029 0.000000 3.970039
He 0.000000 0.000000 0.000000

^{3}He@D_{5h}(1)-C_{70}^{6-}
71

C 0.755011 -2.323684 -3.221095
C 1.982981 -2.323863 -2.451559
C 0.382384 -1.176856 -4.002264
C 2.822900 -1.167814 -2.451559
C 3.447346 -0.737813 -1.224969
C 3.276982 -1.463242 0.000000
C 3.447346 -0.737813 1.224969
C -1.976644 -1.436116 -3.221095
C -1.597350 -2.604040 -2.451559
C -1.001093 -0.727337 -4.002264
C -0.238333 -3.045612 -2.451559
C 0.363586 -3.506617 -1.224969
C -0.378983 -3.568762 0.000000
C 0.363586 -3.506617 1.224969
C 2.404269 -2.664428 0.000000
C 1.766991 -3.050624 -1.224969
C 1.766991 -3.050624 1.224969
C -1.976644 1.436116 -3.221095
C -2.970198 0.714477 -2.451559
C -1.001093 0.727337 -4.002264
C -2.970198 -0.714477 -2.451559
C -3.222637 -1.429395 -1.224969
C -3.511206 -0.742374 0.000000
C -3.222637 -1.429395 1.224969
C -1.791062 -3.109949 0.000000
C -2.355285 -2.623203 -1.224969
C -2.355285 -2.623203 1.224969
C 0.755011 2.323684 -3.221095
C -0.238333 3.045612 -2.451559
C 0.382384 1.176856 -4.002264
C -1.597350 2.604040 -2.451559
C -2.355285 2.623203 -1.224969
C -1.791062 3.109949 0.000000
C -2.355285 2.623203 1.224969
C -3.511206 0.742374 0.000000
C -3.222637 1.429395 -1.224969
C -3.222637 1.429395 1.224969
C 2.443266 0.000000 -3.221095
C 2.822900 1.167814 -2.451559
C 1.237419 0.000000 -4.002264

C	1.982981	2.323863	-2.451559
C	1.766991	3.050624	-1.224969
C	2.404269	2.664428	0.000000
C	1.766991	3.050624	1.224969
C	-0.378983	3.568762	0.000000
C	0.363586	3.506617	-1.224969
C	0.363586	3.506617	1.224969
C	3.276982	1.463242	0.000000
C	3.447346	0.737813	-1.224969
C	3.447346	0.737813	1.224969
C	0.755011	2.323684	3.221095
C	1.982981	2.323863	2.451559
C	2.822900	1.167814	2.451559
C	0.382384	1.176856	4.002264
C	-1.976644	1.436116	3.221095
C	-1.597350	2.604040	2.451559
C	-0.238333	3.045612	2.451559
C	-1.001093	0.727337	4.002264
C	-1.976644	-1.436116	3.221095
C	-2.970198	-0.714477	2.451559
C	-2.970198	0.714477	2.451559
C	-1.001093	-0.727337	4.002264
C	0.755011	-2.323684	3.221095
C	-0.238333	-3.045612	2.451559
C	-1.597350	-2.604040	2.451559
C	0.382384	-1.176856	4.002264
C	2.443266	0.000000	3.221095
C	2.822900	-1.167814	2.451559
C	1.982981	-2.323863	2.451559
C	1.237419	0.000000	4.002264
He	0.000000	0.000000	0.000000

$He@C_{60}^{12-}$
61

C	-1.2508585	0.0000000	3.4425444
C	-0.3865365	-1.1896372	3.4425444
C	1.0119658	-0.7352362	3.4425444
C	1.0119658	0.7352362	3.4425444
C	-0.3865365	1.1896372	3.4425444
C	2.4250202	-2.6706823	0.6344229
C	3.2893422	-1.4810451	0.6344229
C	3.0504495	-0.7458089	1.8852815
C	2.0384837	-1.4810451	2.6583546
C	1.6519471	-2.6706823	1.8852815
C	3.2893422	1.4810451	0.6344229
C	2.4250202	2.6706823	0.6344229
C	1.6519471	2.6706823	1.8852815
C	2.0384837	1.4810451	2.6583546

C	3.0504495	0.7458089	1.8852815
C	-0.3920949	3.5860185	0.6344229
C	-1.7905973	3.1316175	0.6344229
C	-2.0294900	2.3963813	1.8852815
C	-0.7786315	2.3963813	2.6583546
C	0.2333343	3.1316175	1.8852815
C	-3.5316702	0.7352362	0.6344229
C	-3.5316702	-0.7352362	0.6344229
C	-2.9062410	-1.1896372	1.8852815
C	-2.5197044	0.0000000	2.6583546
C	-2.9062410	1.1896372	1.8852815
C	-1.7905973	-3.1316175	0.6344229
C	-0.3920949	-3.5860185	0.6344229
C	0.2333343	-3.1316175	1.8852815
C	-0.7786315	-2.3963813	2.6583546
C	-2.0294900	-2.3963813	1.8852815
C	-0.2333343	-3.1316175	-1.8852815
C	0.7786315	-2.3963813	-2.6583546
C	2.0294900	-2.3963813	-1.8852815
C	1.7905973	-3.1316175	-0.6344229
C	0.3920949	-3.5860185	-0.6344229
C	2.9062410	-1.1896372	-1.8852815
C	2.5197044	0.0000000	-2.6583546
C	2.9062410	1.1896372	-1.8852815
C	3.5316702	0.7352362	-0.6344229
C	3.5316702	-0.7352362	-0.6344229
C	2.0294900	2.3963813	-1.8852815
C	0.7786315	2.3963813	-2.6583546
C	-0.2333343	3.1316175	-1.8852815
C	0.3920949	3.5860185	-0.6344229
C	1.7905973	3.1316175	-0.6344229
C	-1.6519471	2.6706823	-1.8852815
C	-2.0384837	1.4810451	-2.6583546
C	-3.0504495	0.7458089	-1.8852815
C	-3.2893422	1.4810451	-0.6344229
C	-2.4250202	2.6706823	-0.6344229
C	-3.0504495	-0.7458089	-1.8852815
C	-2.0384837	-1.4810451	-2.6583546
C	-1.6519471	-2.6706823	-1.8852815
C	-2.4250202	-2.6706823	-0.6344229
C	-3.2893422	-1.4810451	-0.6344229
C	-1.0119658	-0.7352362	-3.4425444
C	-1.0119658	0.7352362	-3.4425444
C	0.3865365	1.1896372	-3.4425444
C	1.2508585	0.0000000	-3.4425444
C	0.3865365	-1.1896372	-3.4425444
He	0.0000000	0.0000000	0.0000000

$^{3}He@D_{2}(1)\text{-}C_{76}$
77

C	2.494936	2.732426	0.155695
C	2.056021	2.652620	1.494392
C	2.737679	1.708720	2.321460
C	2.100485	1.168194	3.500117
C	0.838892	1.618263	3.859816
C	-0.234543	3.366226	0.694448
C	0.683736	3.051114	1.801846
C	0.141786	2.597878	3.036004
C	-1.619406	3.181394	0.913544
C	-2.131940	2.647391	2.142615
C	-1.267982	2.359543	3.195049
C	0.234543	3.366226	-0.694448
C	-0.683736	3.051114	-1.801846
C	1.619406	3.181394	-0.913544
C	-0.141786	2.597878	-3.036004
C	1.454294	-1.155095	3.983649
C	0.145012	-0.686448	4.386612
C	2.438182	-0.237129	3.599609
C	-0.145012	0.686448	4.386612
C	-1.454294	1.155095	3.983649
C	-0.838892	-1.618263	3.859816
C	-2.100485	-1.168194	3.500117
C	-2.438182	0.237129	3.599609
C	3.221330	-1.746783	1.817636
C	2.131940	-2.647391	2.142615
C	3.332099	-0.536878	2.497823
C	1.267982	-2.359543	3.195049
C	-0.141786	-2.597878	3.036004
C	1.619406	-3.181394	0.913544
C	0.234543	-3.366226	0.694448
C	-0.683736	-3.051114	1.801846
C	-2.056021	-2.652620	1.494392
C	-2.494936	-2.732426	0.155695
C	-2.737679	-1.708720	2.321460
C	3.556602	-0.680758	-1.738586
C	3.829065	-0.647678	-0.346077
C	3.438832	-1.802254	0.393510
C	2.494936	-2.732426	-0.155695
C	2.056021	-2.652620	-1.494392
C	2.737679	-1.708720	-2.321460
C	0.838892	-1.618263	-3.859816
C	2.100485	-1.168194	-3.500117
C	-1.619406	-3.181394	-0.913544
C	-0.234543	-3.366226	-0.694448
C	0.683736	-3.051114	-1.801846
C	0.141786	-2.597878	-3.036004
C	3.829065	0.647678	0.346077
C	3.556602	0.680758	1.738586
C	3.332099	0.536878	-2.497823
C	3.221330	1.746783	-1.817636
C	3.438832	1.802254	-0.393510

C 2.438182 0.237129 -3.599609
C 2.131940 2.647391 -2.142615
C 1.267982 2.359543 -3.195049
C 1.454294 1.155095 -3.983649
C -1.454294 -1.155095 -3.983649
C -0.145012 -0.686448 -4.386612
C 0.145012 0.686448 -4.386612
C -2.438182 -0.237129 -3.599609
C -3.221330 -1.746783 -1.817636
C -2.131940 -2.647391 -2.142615
C -1.267982 -2.359543 -3.195049
C -3.332099 -0.536878 -2.497823
C -3.556602 -0.680758 1.738586
C -3.829065 -0.647678 0.346077
C -3.438832 -1.802254 -0.393510
C -3.438832 1.802254 0.393510
C -3.221330 1.746783 1.817636
C -3.332099 0.536878 2.497823
C -3.556602 0.680758 -1.738586
C -3.829065 0.647678 -0.346077
C -0.838892 1.618263 -3.859816
C -2.100485 1.168194 -3.500117
C -2.737679 1.708720 -2.321460
C -2.056021 2.652620 -1.494392
C -2.494936 2.732426 -0.155695
He 0.000000 0.000000 0.000000

$^{3}He@D_{2}(1)\text{-}C_{76}^{6-}$

77

C 2.508492 2.778565 0.147598
C 2.058321 2.682920 1.492218
C 2.750385 1.744396 2.342531
C 2.105282 1.185335 3.500094
C 0.823963 1.635461 3.879048
C -0.233405 3.394291 0.695316
C 0.683149 3.075411 1.800783
C 0.134237 2.622234 3.064285
C -1.645199 3.209773 0.915831
C -2.152607 2.639343 2.147238
C -1.277677 2.351730 3.209067
C 0.233405 3.394291 -0.695316
C -0.683149 3.075411 -1.800783
C 1.645199 3.209773 -0.915831
C -0.134237 2.622234 -3.064285
C 1.462220 -1.158066 4.024603
C 0.158744 -0.706199 4.431505
C 2.482369 -0.217808 3.626628
C -0.158744 0.706199 4.431505
C -1.462220 1.158066 4.024603
C -0.823963 -1.635461 3.879048
C -2.105282 -1.185335 3.500094

C	-2.482369	0.217808	3.626628
C	3.254639	-1.755244	1.827578
C	2.152607	-2.639343	2.147238
C	3.369604	-0.513541	2.535307
C	1.277677	-2.351730	3.209067
C	-0.134237	-2.622234	3.064285
C	1.645199	-3.209773	0.915831
C	0.233405	-3.394291	0.695316
C	-0.683149	-3.075411	1.800783
C	-2.058321	-2.682920	1.492218
C	-2.508492	-2.778565	0.147598
C	-2.750385	-1.744396	2.342531
C	3.579232	-0.692666	-1.754431
C	3.835537	-0.651552	-0.349046
C	3.466624	-1.815358	0.412429
C	2.508492	-2.778565	-0.147598
C	2.058321	-2.682920	-1.492218
C	2.750385	-1.744396	-2.342531
C	0.823963	-1.635461	-3.879048
C	2.105282	-1.185335	-3.500094
C	-1.645199	-3.209773	-0.915831
C	-0.233405	-3.394291	-0.695316
C	0.683149	-3.075411	-1.800783
C	0.134237	-2.622234	-3.064285
C	3.835537	0.651552	0.349046
C	3.579232	0.692666	1.754431
C	3.369604	0.513541	-2.535307
C	3.254639	1.755244	-1.827578
C	3.466624	1.815358	-0.412429
C	2.482369	0.217808	-3.626628
C	2.152607	2.639343	-2.147238
C	1.277677	2.351730	-3.209067
C	1.462220	1.158066	-4.024603
C	-1.462220	-1.158066	-4.024603
C	-0.158744	-0.706199	-4.431505
C	0.158744	0.706199	-4.431505
C	-2.482369	-0.217808	-3.626628
C	-3.254639	-1.755244	-1.827578
C	-2.152607	-2.639343	-2.147238
C	-1.277677	-2.351730	-3.209067
C	-3.369604	-0.513541	-2.535307
C	-3.579232	-0.692666	1.754431
C	-3.835537	-0.651552	0.349046
C	-3.466624	-1.815358	-0.412429
C	-3.466624	1.815358	0.412429
C	-3.254639	1.755244	1.827578
C	-3.369604	0.513541	2.535307
C	-3.579232	0.692666	-1.754431
C	-3.835537	0.651552	-0.349046
C	-0.823963	1.635461	-3.879048
C	-2.105282	1.185335	-3.500094

C -2.750385 1.744396 -2.342531
C -2.058321 2.682920 -1.492218
C -2.508492 2.778565 -0.147598
He 0.000000 0.000000 0.000000

^{3}He@C_{2v}(3)-C_{78}
79

C -4.2203308 0.7024274 -1.1786338
C -3.4209249 1.4167659 -2.1526726
C -4.2203308 -0.7024274 -1.1786338
C -2.7195808 0.7269888 -3.1315672
C -0.7300994 3.6232641 -0.8608514
C -2.7842771 2.5404005 -1.5010243
C -1.4670668 2.9622493 -1.8725894
C -0.7363867 2.2557879 -2.9287531
C 0.7363867 2.2557879 -2.9287531
C -1.4109792 1.1764973 -3.5571238
C 1.4109792 1.1764973 -3.5571238
C -4.0652503 -0.7247791 1.2708446
C -4.0652503 0.7247791 1.2708446
C -4.1124124 -1.4220479 0.0669329
C -4.1124124 1.4220479 0.0669329
C -3.2261767 2.5612679 -0.1307567
C -2.3802638 3.0250714 0.9093797
C -1.1828650 3.6782315 0.4883923
C -1.1844819 -2.3563407 2.9936794
C -2.3785923 -2.3211314 2.2006365
C -3.2005603 -1.1719419 2.3423626
C -2.7208138 0.0000000 3.0342254
C -0.7321730 1.2237842 3.7223276
C -1.4598012 0.0000000 3.7007721
C -0.7321730 -1.2237842 3.7223276
C -2.3785923 2.3211314 2.2006365
C -3.2005603 1.1719419 2.3423626
C -1.1844819 2.3563407 2.9936794
C -2.3802638 -3.0250714 0.9093797
C -3.2261767 -2.5612679 -0.1307567
C 0.0000000 -3.0623011 2.5453930
C 0.0000000 -3.6993809 1.3226193
C -1.1828650 -3.6782315 0.4883923
C 1.1844819 -2.3563407 2.9936794
C 2.3785923 -2.3211314 2.2006365
C 3.2005603 -1.1719419 2.3423626
C 0.7321730 1.2237842 3.7223276
C 1.4598012 0.0000000 3.7007721
C 0.7321730 -1.2237842 3.7223276
C 2.7208138 0.0000000 3.0342254
C -0.7300994 -3.6232641 -0.8608514
C -1.4670668 -2.9622493 -1.8725894
C -2.7842771 -2.5404005 -1.5010243

C	-3.4209249	-1.4167659	-2.1526726
C	-2.7195808	-0.7269888	-3.1315672
C	0.7363867	-2.2557879	-2.9287531
C	-0.7363867	-2.2557879	-2.9287531
C	-1.4109792	-1.1764973	-3.5571238
C	1.4109792	-1.1764973	-3.5571238
C	0.6881402	0.0000000	-3.9610292
C	-0.6881402	0.0000000	-3.9610292
C	0.7300994	-3.6232641	-0.8608514
C	2.7842771	-2.5404005	-1.5010243
C	1.4670668	-2.9622493	-1.8725894
C	2.3802638	-3.0250714	0.9093797
C	1.1828650	-3.6782315	0.4883923
C	3.2261767	-2.5612679	-0.1307567
C	4.2203308	-0.7024274	-1.1786338
C	3.4209249	-1.4167659	-2.1526726
C	2.7195808	-0.7269888	-3.1315672
C	4.2203308	0.7024274	-1.1786338
C	4.0652503	0.7247791	1.2708446
C	4.0652503	-0.7247791	1.2708446
C	4.1124124	-1.4220479	0.0669329
C	4.1124124	1.4220479	0.0669329
C	1.1844819	2.3563407	2.9936794
C	2.3785923	2.3211314	2.2006365
C	3.2005603	1.1719419	2.3423626
C	1.1828650	3.6782315	0.4883923
C	0.0000000	3.6993809	1.3226193
C	0.0000000	3.0623011	2.5453930
C	3.2261767	2.5612679	-0.1307567
C	2.3802638	3.0250714	0.9093797
C	2.7195808	0.7269888	-3.1315672
C	3.4209249	1.4167659	-2.1526726
C	2.7842771	2.5404005	-1.5010243
C	1.4670668	2.9622493	-1.8725894
C	0.7300994	3.6232641	-0.8608514
He	0.0000000	0.0000000	-0.0062950

^{3}He@C_{2v}(3)-C_{78}^{6-}
79

C	-4.2232777	0.7241387	-1.1956839
C	-3.4238861	1.4292110	-2.1654995
C	-4.2232777	-0.7241387	-1.1956839
C	-2.7097489	0.7372374	-3.1748378
C	-0.7153111	3.6781023	-0.8814659
C	-2.7809377	2.5618442	-1.5211131
C	-1.4612182	2.9862573	-1.8903966
C	-0.7269984	2.2963926	-2.9625710
C	0.7269984	2.2963926	-2.9625710
C	-1.4304019	1.1950357	-3.6197941
C	1.4304019	1.1950357	-3.6197941

C	-4.0523853	-0.7278566	1.2916277
C	-4.0523853	0.7278566	1.2916277
C	-4.0938285	-1.4341469	0.0583289
C	-4.0938285	1.4341469	0.0583289
C	-3.2251852	2.5771437	-0.1305331
C	-2.3627160	3.0404113	0.9206488
C	-1.1703419	3.7240231	0.5063757
C	-1.1738362	-2.3946629	3.0249239
C	-2.3631041	-2.3416585	2.2161190
C	-3.2037763	-1.1789247	2.3644643
C	-2.7239997	0.0000000	3.0770889
C	-0.7201233	1.2326145	3.7788244
C	-1.4590256	0.0000000	3.7335154
C	-0.7201233	-1.2326145	3.7788244
C	-2.3631041	2.3416585	2.2161190
C	-3.2037763	1.1789247	2.3644643
C	-1.1738362	2.3946629	3.0249239
C	-2.3627160	-3.0404113	0.9206488
C	-3.2251852	-2.5771437	-0.1305331
C	0.0000000	-3.1104509	2.5961524
C	-0.0000000	-3.7685096	1.3383531
C	-1.1703419	-3.7240231	0.5063757
C	1.1738362	-2.3946629	3.0249239
C	2.3631041	-2.3416585	2.2161190
C	3.2037763	-1.1789247	2.3644643
C	0.7201233	1.2326145	3.7788244
C	1.4590256	0.0000000	3.7335154
C	0.7201233	-1.2326145	3.7788244
C	2.7239997	0.0000000	3.0770889
C	-0.7153111	-3.6781023	-0.8814659
C	-1.4612182	-2.9862573	-1.8903966
C	-2.7809377	-2.5618442	-1.5211131
C	-3.4238861	-1.4292110	-2.1654995
C	-2.7097489	-0.7372374	-3.1748378
C	0.7269984	-2.2963926	-2.9625710
C	-0.7269984	-2.2963926	-2.9625710
C	-1.4304019	-1.1950357	-3.6197941
C	1.4304019	-1.1950357	-3.6197941
C	0.6883005	0.0000000	-3.9806847
C	-0.6883005	0.0000000	-3.9806847
C	0.7153111	-3.6781023	-0.8814659
C	2.7809377	-2.5618442	-1.5211131
C	1.4612182	-2.9862573	-1.8903966
C	2.3627160	-3.0404113	0.9206488
C	1.1703419	-3.7240231	0.5063757
C	3.2251852	-2.5771437	-0.1305331
C	4.2232777	-0.7241387	-1.1956839
C	3.4238861	-1.4292110	-2.1654995
C	2.7097489	-0.7372374	-3.1748378
C	4.2232777	0.7241387	-1.1956839
C	4.0523853	0.7278566	1.2916277

C 4.0523853 -0.7278566 1.2916277
C 4.0938285 -1.4341469 0.0583289
C 4.0938285 1.4341469 0.0583289
C 1.1738362 2.3946629 3.0249239
C 2.3631041 2.3416585 2.2161190
C 3.2037763 1.1789247 2.3644643
C 1.1703419 3.7240231 0.5063757
C -0.0000000 3.7685096 1.3383531
C 0.0000000 3.1104509 2.5961524
C 3.2251852 2.5771437 -0.1305331
C 2.3627160 3.0404113 0.9206488
C 2.7097489 0.7372374 -3.1748378
C 3.4238861 1.4292110 -2.1654995
C 2.7809377 2.5618442 -1.5211131
C 1.4612182 2.9862573 -1.8903966
C 0.7153111 3.6781023 -0.8814659
He 0.0000000 0.0000000 -0.0065209

^{3}He@C_{2v}(2)-C_{78}

79

C 4.297455 0.720081 1.173464
C 3.451155 1.156567 2.274434
C 4.256114 1.420562 -0.041708
C 2.719780 2.325637 2.169366
C 1.405290 2.401555 2.744727
C 4.147891 -0.696067 -1.289438
C 4.256114 -1.420562 -0.041708
C 4.147891 0.696067 -1.289438
C 4.297455 -0.720081 1.173464
C 3.451155 -1.156567 2.274434
C 3.430783 -2.604756 -0.166608
C 2.721152 -3.082872 0.924212
C 2.719780 -2.325637 2.169366
C 2.842831 0.000000 2.893722
C 1.474527 0.000000 3.319698
C 0.734480 1.261491 3.276638
C 1.180161 -1.413626 -3.422137
C 2.380623 -0.735123 -3.064369
C 3.234810 -1.421402 -2.162139
C 1.466340 -3.121079 -1.640538
C 0.727715 -2.568802 -2.715539
C 2.787831 -2.595922 -1.463059
C 2.380623 0.735123 -3.064369
C 3.234810 1.421402 -2.162139
C 0.000000 -0.690719 -3.843653
C 0.000000 0.690719 -3.843653
C 1.180161 1.413626 -3.422137
C -1.180161 -1.413626 -3.422137
C -2.380623 -0.735123 -3.064369
C -3.234810 -1.421402 -2.162139
C -1.466340 -3.121079 -1.640538

C	-0.727715	-2.568802	-2.715539
C	-2.787831	-2.595922	-1.463059
C	-0.735496	-3.675498	-0.497905
C	1.409010	-3.661834	0.753608
C	0.735496	-3.675498	-0.497905
C	-1.409010	-3.661834	0.753608
C	0.727715	2.568802	-2.715539
C	1.466340	3.121079	-1.640538
C	2.787831	2.595922	-1.463059
C	3.430783	2.604756	-0.166608
C	2.721152	3.082872	0.924212
C	-0.735496	3.675498	-0.497905
C	0.735496	3.675498	-0.497905
C	1.409010	3.661834	0.753608
C	-1.409010	3.661834	0.753608
C	-0.684591	3.373888	1.962070
C	0.684591	3.373888	1.962070
C	-0.727715	2.568802	-2.715539
C	-2.787831	2.595922	-1.463059
C	-1.466340	3.121079	-1.640538
C	-2.380623	0.735123	-3.064369
C	-1.180161	1.413626	-3.422137
C	-3.234810	1.421402	-2.162139
C	-4.256114	1.420562	-0.041708
C	-3.430783	2.604756	-0.166608
C	-2.721152	3.082872	0.924212
C	-4.297455	0.720081	1.173464
C	-4.256114	-1.420562	-0.041708
C	-4.147891	-0.696067	-1.289438
C	-4.147891	0.696067	-1.289438
C	-4.297455	-0.720081	1.173464
C	-2.719780	-2.325637	2.169366
C	-2.721152	-3.082872	0.924212
C	-3.430783	-2.604756	-0.166608
C	-3.451155	-1.156567	2.274434
C	0.684591	-3.373888	1.962070
C	-1.405290	-2.401555	2.744727
C	-0.684591	-3.373888	1.962070
C	-2.719780	2.325637	2.169366
C	-1.405290	2.401555	2.744727
C	-0.734480	1.261491	3.276638
C	-3.451155	1.156567	2.274434
C	-2.842831	0.000000	2.893722
C	-1.474527	0.000000	3.319698
C	-0.734480	-1.261491	3.276638
C	0.734480	-1.261491	3.276638
C	1.405290	-2.401555	2.744727
He	0.000000	0.000000	-0.065672

^{3}He@C_{2v}(2)-C_{78}^{4-}

C	4.310317	0.716336	1.176474
C	3.455707	1.155353	2.268963
C	4.268401	1.442448	-0.056769
C	2.718599	2.332221	2.167806
C	1.407015	2.407092	2.758184
C	4.139116	-0.707783	-1.303572
C	4.268401	-1.442448	-0.056769
C	4.139116	0.707783	-1.303572
C	4.310317	-0.716336	1.176474
C	3.455707	-1.155353	2.268963
C	3.446401	-2.619925	-0.172210
C	2.725672	-3.114885	0.936329
C	2.718599	-2.332221	2.167806
C	2.846501	0.000000	2.901264
C	1.476885	0.000000	3.337656
C	0.733223	1.261210	3.299478
C	1.169874	-1.416797	-3.444859
C	2.366836	-0.733679	-3.072795
C	3.239811	-1.426524	-2.169948
C	1.466820	-3.132820	-1.636031
C	0.715476	-2.596868	-2.723440
C	2.792771	-2.618782	-1.464519
C	2.366836	0.733679	-3.072795
C	3.239811	1.426524	-2.169948
C	0.000000	-0.706088	-3.880595
C	0.000000	0.706088	-3.880595
C	1.169874	1.416797	-3.444859
C	-1.169874	-1.416797	-3.444859
C	-2.366836	-0.733679	-3.072795
C	-3.239811	-1.426524	-2.169948
C	-1.466820	-3.132820	-1.636031
C	-0.715476	-2.596868	-2.723440
C	-2.792771	-2.618782	-1.464519
C	-0.731630	-3.696025	-0.493291
C	1.428487	-3.697087	0.772524
C	0.731630	-3.696025	-0.493291
C	-1.428487	-3.697087	0.772524
C	0.715476	2.596868	-2.723440
C	1.466820	3.132820	-1.636031
C	2.792771	2.618782	-1.464519
C	3.446401	2.619925	-0.172210
C	2.725672	3.114885	0.936329
C	-0.731630	3.696025	-0.493291
C	0.731630	3.696025	-0.493291
C	1.428487	3.697087	0.772524
C	-1.428487	3.697087	0.772524
C	-0.684357	3.380761	1.976359
C	0.684357	3.380761	1.976359
C	-0.715476	2.596868	-2.723440
C	-2.792771	2.618782	-1.464519

C -1.466820 3.132820 -1.636031
C -2.366836 0.733679 -3.072795
C -1.169874 1.416797 -3.444859
C -3.239811 1.426524 -2.169948
C -4.268401 1.442448 -0.056769
C -3.446401 2.619925 -0.172210
C -2.725672 3.114885 0.936329
C -4.310317 0.716336 1.176474
C -4.268401 -1.442448 -0.056769
C -4.139116 -0.707783 -1.303572
C -4.139116 0.707783 -1.303572
C -4.310317 -0.716336 1.176474
C -2.718599 -2.332221 2.167806
C -2.725672 -3.114885 0.936329
C -3.446401 -2.619925 -0.172210
C -3.455707 -1.155353 2.268963
C 0.684357 -3.380761 1.976359
C -1.407015 -2.407092 2.758184
C -0.684357 -3.380761 1.976359
C -2.718599 2.332221 2.167806
C -1.407015 2.407092 2.758184
C -0.733223 1.261210 3.299478
C -3.455707 1.155353 2.268963
C -2.846501 0.000000 2.901264
C -1.476885 0.000000 3.337656
C -0.733223 -1.261210 3.299478
C 0.733223 -1.261210 3.299478
C 1.407015 -2.407092 2.758184
He 0.000000 0.000000 -0.023514
^{3}He@D_2(22)C_{84}
85

C 1.8491708 2.8103378 -2.5881277
C -1.8491708 -2.8103378 -2.5881277
C 1.8491708 -2.8103378 2.5881277
C -1.8491708 2.8103378 2.5881277
C 2.2232790 1.5948981 -3.2491144
C -2.2232790 -1.5948981 -3.2491144
C 2.2232790 -1.5948981 3.2491144
C -2.2232790 1.5948981 3.2491144
C 3.2865029 0.8664422 -2.6391387
C -3.2865029 -0.8664422 -2.6391387
C 3.2865029 -0.8664422 2.6391387
C -3.2865029 0.8664422 2.6391387
C 2.3501153 3.1557694 -1.2889386
C -2.3501153 -3.1557694 -1.2889386
C 2.3501153 -3.1557694 1.2889386
C -2.3501153 3.1557694 1.2889386
C 3.3036715 2.3483198 -0.6063467
C -3.3036715 -2.3483198 -0.6063467
C 3.3036715 -2.3483198 0.6063467

C	-3.3036715	2.3483198	0.6063467
C	3.8300235	1.2445604	-1.3612913
C	-3.8300235	-1.2445604	-1.3612913
C	3.8300235	-1.2445604	1.3612913
C	-3.8300235	1.2445604	1.3612913
C	1.1996366	0.8618370	-4.0185667
C	-1.1996366	-0.8618370	-4.0185667
C	1.1996366	-0.8618370	4.0185667
C	-1.1996366	0.8618370	4.0185667
C	1.2905745	-0.5633631	-4.1083085
C	-1.2905745	0.5633631	-4.1083085
C	1.2905745	0.5633631	4.1083085
C	-1.2905745	-0.5633631	4.1083085
C	0.4862603	3.3048152	-2.6587567
C	-0.4862603	-3.3048152	-2.6587567
C	0.4862603	-3.3048152	2.6587567
C	-0.4862603	3.3048152	2.6587567
C	-0.4749585	2.6259414	-3.3888753
C	0.4749585	-2.6259414	-3.3888753
C	-0.4749585	-2.6259414	3.3888753
C	0.4749585	2.6259414	3.3888753
C	-0.1248888	1.4017602	-4.0988223
C	0.1248888	-1.4017602	-4.0988223
C	-0.1248888	-1.4017602	4.0988223
C	0.1248888	1.4017602	4.0988223
C	0.1268704	3.9091352	-1.3937711
C	-0.1268704	-3.9091352	-1.3937711
C	0.1268704	-3.9091352	1.3937711
C	-0.1268704	3.9091352	1.3937711
C	-1.1972966	3.7672225	-0.8570016
C	1.1972966	-3.7672225	-0.8570016
C	-1.1972966	-3.7672225	0.8570016
C	1.1972966	3.7672225	0.8570016
C	-1.2928113	3.8494022	0.5567911
C	1.2928113	-3.8494022	0.5567911
C	-1.2928113	-3.8494022	-0.5567911
C	1.2928113	3.8494022	-0.5567911
C	2.2111358	3.0018149	1.6006869
C	-2.2111358	-3.0018149	1.6006869
C	2.2111358	-3.0018149	-1.6006869
C	-2.2111358	3.0018149	-1.6006869
C	3.8323415	1.1228852	1.4774049
C	-3.8323415	-1.1228852	1.4774049
C	3.8323415	-1.1228852	-1.4774049
C	-3.8323415	1.1228852	-1.4774049
C	3.2594827	2.2785790	0.8640698
C	-3.2594827	-2.2785790	0.8640698
C	3.2594827	-2.2785790	-0.8640698
C	-3.2594827	2.2785790	-0.8640698
C	1.8403896	2.5200696	2.8930019
C	-1.8403896	-2.5200696	2.8930019

C 1.8403896 -2.5200696 -2.8930019
C -1.8403896 2.5200696 -2.8930019
C -2.3583556 1.2853882 -3.4225057
C 2.3583556 -1.2853882 -3.4225057
C -2.3583556 -1.2853882 3.4225057
C 2.3583556 1.2853882 3.4225057
C -3.3328006 0.5899070 -2.7186666
C 3.3328006 -0.5899070 -2.7186666
C -3.3328006 -0.5899070 2.7186666
C 3.3328006 0.5899070 2.7186666
C 4.2445694 -0.0268942 0.6901315
C -4.2445694 0.0268942 0.6901315
C 4.2445694 0.0268942 -0.6901315
C -4.2445694 -0.0268942 -0.6901315
He 0.0000000 0.0000000 0.0000000

$^{3}He@D_{2}(22)C_{84}^{6-}$
85

C 1.8495751 2.8458988 -2.6044524
C -1.8495751 -2.8458988 -2.6044524
C 1.8495751 -2.8458988 2.6044524
C -1.8495751 2.8458988 2.6044524
C 2.2196345 1.6119381 -3.2532189
C -2.2196345 -1.6119381 -3.2532189
C 2.2196345 -1.6119381 3.2532189
C -2.2196345 1.6119381 3.2532189
C 3.3004063 0.8811391 -2.6547315
C -3.3004063 -0.8811391 -2.6547315
C 3.3004063 -0.8811391 2.6547315
C -3.3004063 0.8811391 2.6547315
C 2.3620021 3.1881757 -1.2699702
C -2.3620021 -3.1881757 -1.2699702
C 2.3620021 -3.1881757 1.2699702
C -2.3620021 3.1881757 1.2699702
C 3.3150039 2.3620858 -0.5878431
C -3.3150039 -2.3620858 -0.5878431
C 3.3150039 -2.3620858 0.5878431
C -3.3150039 2.3620858 0.5878431
C 3.8719897 1.2639502 -1.3590266
C -3.8719897 -1.2639502 -1.3590266
C 3.8719897 -1.2639502 1.3590266
C -3.8719897 1.2639502 1.3590266
C 1.1980729 0.8762876 -4.0432096
C -1.1980729 -0.8762876 -4.0432096
C 1.1980729 -0.8762876 4.0432096
C -1.1980729 0.8762876 4.0432096
C 1.3172522 -0.5606300 -4.1711996
C -1.3172522 0.5606300 -4.1711996
C 1.3172522 0.5606300 4.1711996
C -1.3172522 -0.5606300 4.1711996
C 0.4962536 3.3331727 -2.6775018

C	-0.4962536	-3.3331727	-2.6775018
C	0.4962536	-3.3331727	2.6775018
C	-0.4962536	3.3331727	2.6775018
C	-0.4833102	2.6385368	-3.4392404
C	0.4833102	-2.6385368	-3.4392404
C	-0.4833102	-2.6385368	3.4392404
C	0.4833102	2.6385368	3.4392404
C	-0.1243115	1.4269346	-4.1471034
C	0.1243115	-1.4269346	-4.1471034
C	-0.1243115	-1.4269346	4.1471034
C	0.1243115	1.4269346	4.1471034
C	0.1308379	3.9218501	-1.4153312
C	-0.1308379	-3.9218501	-1.4153312
C	0.1308379	-3.9218501	1.4153312
C	-0.1308379	3.9218501	1.4153312
C	-1.2000897	3.7652107	-0.8754144
C	1.2000897	-3.7652107	-0.8754144
C	-1.2000897	-3.7652107	0.8754144
C	1.2000897	3.7652107	0.8754144
C	-1.3128381	3.8636898	0.5509961
C	1.3128381	-3.8636898	0.5509961
C	-1.3128381	-3.8636898	-0.5509961
C	1.3128381	3.8636898	-0.5509961
C	2.2107933	2.9968623	1.6210958
C	-2.2107933	-2.9968623	1.6210958
C	2.2107933	-2.9968623	-1.6210958
C	-2.2107933	2.9968623	-1.6210958
C	3.8552545	1.1043303	1.5054775
C	-3.8552545	-1.1043303	1.5054775
C	3.8552545	-1.1043303	-1.5054775
C	-3.8552545	1.1043303	-1.5054775
C	3.2615735	2.2786866	0.8820798
C	-3.2615735	-2.2786866	0.8820798
C	3.2615735	-2.2786866	-0.8820798
C	-3.2615735	2.2786866	-0.8820798
C	1.8364347	2.5173405	2.9434198
C	-1.8364347	-2.5173405	2.9434198
C	1.8364347	-2.5173405	-2.9434198
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C	-2.3579490	1.2666271	-3.4714012
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C	-2.3579490	-1.2666271	3.4714012
C	2.3579490	1.2666271	3.4714012
C	-3.3469546	0.5659350	-2.7428697
C	3.3469546	-0.5659350	-2.7428697
C	-3.3469546	-0.5659350	2.7428697
C	3.3469546	0.5659350	2.7428697
C	4.2597527	-0.0402021	0.7031171
C	-4.2597527	0.0402021	0.7031171
C	4.2597527	0.0402021	-0.7031171
C	-4.2597527	-0.0402021	-0.7031171

He 0.0000000 0.0000000 0.0000000

^{3}He@D_{2d}(4)C_{84}
85

C -2.0872456 -3.1001285 -1.3663648
C 2.0872456 3.1001285 -1.3663648
C -2.0872456 3.1001285 1.3663648
C 2.0872456 -3.1001285 1.3663648
C -1.0731918 -3.1352015 -2.3485287
C 1.0731918 3.1352015 -2.3485287
C -1.0731918 3.1352015 2.3485287
C 1.0731918 -3.1352015 2.3485287
C -1.2844785 -2.3066442 -3.4887414
C 1.2844785 2.3066442 -3.4887414
C -1.2844785 2.3066442 3.4887414
C 1.2844785 -2.3066442 3.4887414
C -0.1771282 -1.8264808 -4.2769651
C 0.1771282 1.8264808 -4.2769651
C -0.1771282 1.8264808 4.2769651
C 0.1771282 -1.8264808 4.2769651
C 1.1178191 -2.1457188 -3.8785934
C -1.1178191 2.1457188 -3.8785934
C 1.1178191 2.1457188 3.8785934
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C 0.5436782 -3.7467469 -0.4913289
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C 0.5436782 3.7467469 0.4913289
C -0.5436782 -3.7467469 0.4913289
C 0.2795995 -3.4812937 -1.9202927
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C 0.2795995 3.4812937 1.9202927
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C 1.3421602 -3.0056857 -2.7351636
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C -1.8434508 -3.4922058 0.0010656
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C -1.8264808 -0.1771282 -4.2769651

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C -1.8264808 0.1771282 4.2769651
C -0.4938636 -0.4938636 -4.7500045
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C 0.4938636 -0.4938636 4.7500045
C 2.1457188 -1.1178191 -3.8785934
C -2.1457188 1.1178191 -3.8785934
C 2.1457188 1.1178191 3.8785934
C -2.1457188 -1.1178191 3.8785934
C 3.1001285 2.0872456 -1.3663648
C -3.1001285 -2.0872456 -1.3663648
C 3.1001285 -2.0872456 1.3663648
C -3.1001285 2.0872456 1.3663648
C 2.3066442 1.2844785 -3.4887414
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C 2.3066442 -1.2844785 3.4887414
C -2.3066442 1.2844785 3.4887414
C 3.1352015 1.0731918 -2.3485287
C -3.1352015 -1.0731918 -2.3485287
C 3.1352015 -1.0731918 2.3485287
C -3.1352015 1.0731918 2.3485287
C 3.4812937 -0.2795995 -1.9202927
C -3.4812937 0.2795995 -1.9202927
C 3.4812937 0.2795995 1.9202927
C -3.4812937 -0.2795995 1.9202927
C 3.7467469 -0.5436782 -0.4913289
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C 3.0056857 -1.3421602 -2.7351636
C -3.0056857 1.3421602 -2.7351636
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C 3.4922058 -1.8434508 -0.0010656
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C 3.4922058 1.8434508 0.0010656
C -3.4922058 -1.8434508 0.0010656
He -0.0000000 0.0000000 0.0000000

$^{3}He@D_{2d}(4)C_{84}^{6-}$

85

C -2.1116772 -3.1511888 -1.3522795
C 2.1116772 3.1511888 -1.3522795
C -2.1116772 3.1511888 1.3522795
C 2.1116772 -3.1511888 1.3522795
C -1.0847110 -3.1597687 -2.3378016
C 1.0847110 3.1597687 -2.3378016
C -1.0847110 3.1597687 2.3378016
C 1.0847110 -3.1597687 2.3378016
C -1.3030104 -2.3336385 -3.4916770

C	1.3030104	2.3336385	-3.4916770
C	-1.3030104	2.3336385	3.4916770
C	1.3030104	-2.3336385	3.4916770
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