

SUPPLEMENTARY TABLE 2

Towards a Global Analysis Method Based on
Anharmonic Ladder Operators: Application to Hydrogen Sulfide
(H₂³²S)

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Supplementary Table 2.

Full calculated rovibrational spectrum of Hydrogen Sulfide up to polyad P=2 and J=20. Rovibrational Hamiltonian parameter values are given in Table 5 of the article.

The available experimental data are included. Energies are sorted by polyad, angular momentum, and symmetry.

First two columns for each level provide the major squared components in the normal basis as well as the quantum numbers for the basis states.

The basis states, (ν_1 , ν_2 , ν_3 , J , K), are denoted by three vibrational normal quantum numbers, ν_1 and ν_3 denote the symmetric and antisymmetric stretching and ν_2 the vibrational bending, the rotational angular momentum J , and its projection $K = |k_a|$. The normal basis components in case of those eigenstates which exhibit a strong coupling among several levels are not explicitly included.

The columns denoted by Eexp, Ecalc, and Residual include the experimental and calculated term values, and the difference between them (units of cm^{-1}). In case the experimental value is lacking, both Eexp and Residual are zero.

POLYAD P = 0

SYMMETRY A2				
EIGENSTATE		Eexp	Ecalc	Residual
		15.0901	15.0901	0.0000
1.000	(0 0 0 1 1)			

SYMMETRY B1				
EIGENSTATE		Eexp	Ecalc	Residual
		13.7463	13.7463	0.0000
1.000	(0 0 0 1 0)			

SYMMETRY B2				
EIGENSTATE		Eexp	Ecalc	Residual
		19.3756	19.3756	0.0001
1.000	(0 0 0 1 1)			

SYMMETRY A1				
EIGENSTATE		Eexp	Ecalc	Residual
		38.0161	38.0161	0.0000
0.842	(0 0 0 2 0)			
		58.3688	58.3687	0.0002
0.842	(0 0 0 2 2)			

SYMMETRY A2				
	EIGENSTATE	Eexp	Ecalc	Residual
	51.1402	51.1400	0.0002	
1.000	(0 0 0 2 1)			

SYMMETRY B1				
	EIGENSTATE	Eexp	Ecalc	Residual
	55.1616	55.1614	0.0001	
1.000	(0 0 0 2 2)			

SYMMETRY B2				
	EIGENSTATE	Eexp	Ecalc	Residual
	38.2978	38.2977	0.0000	
1.000	(0 0 0 2 1)			

SYMMETRY A1				
	EIGENSTATE	Eexp	Ecalc	Residual
	96.3925	96.3921	0.0004	
1.000	(0 0 0 3 2)			

SYMMETRY A2				
	EIGENSTATE	Eexp	Ecalc	Residual
	71.4651	71.4651	0.0000	
0.963	(0 0 0 3 1)			
	115.3406	115.3404	0.0002	
0.963	(0 0 0 3 3)			

SYMMETRY B1				
	EIGENSTATE	Eexp	Ecalc	Residual
	71.4243	71.4243	0.0000	
0.695	(0 0 0 3 0)			
0.305	(0 0 0 3 2)			
	107.3682	107.3679	0.0003	
0.305	(0 0 0 3 0)			
0.695	(0 0 0 3 2)			

SYMMETRY B2				
	EIGENSTATE	Eexp	Ecalc	Residual
	95.0563	95.0562	0.0001	
0.836	(0 0 0 3 1)			
	117.3920	117.3917	0.0002	
0.836	(0 0 0 3 3)			

SYMMETRY A1				
	EIGENSTATE	Eexp	Ecalc	Residual
	114.1722	114.1722	-0.0001	
0.601	(0 0 0 4 0)			
0.391	(0 0 0 4 2)			
	170.3357	170.3357	0.0000	
0.373	(0 0 0 4 0)			
0.500	(0 0 0 4 2)			
	196.8021	196.8020	0.0002	

0.865 (0 0 0 4 4)

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
148.1406	148.1404	0.0002	
0.596 (0 0 0 4 1)			
0.404 (0 0 0 4 3)			
182.6485	182.6481	0.0004	
0.404 (0 0 0 4 1)			
0.596 (0 0 0 4 3)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
148.4183	148.4180	0.0004	
0.939 (0 0 0 4 2)			
195.6614	195.6613	0.0001	
0.939 (0 0 0 4 4)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
114.1776	114.1776	-0.0001	
0.912 (0 0 0 4 1)			
173.9673	173.9666	0.0007	
0.912 (0 0 0 4 3)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
210.2648	210.2644	0.0004	
0.843 (0 0 0 5 2)			
271.1060	271.1050	0.0010	
0.843 (0 0 0 5 4)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
166.3442	166.3443	-0.0001	
0.862 (0 0 0 5 1)			
244.3925	244.3918	0.0007	
0.795 (0 0 0 5 3)			
296.1044	296.1046	-0.0002	
0.927 (0 0 0 5 5)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
166.3434	166.3436	-0.0001	
0.538 (0 0 0 5 0)			
0.438 (0 0 0 5 2)			
243.3434	243.3434	0.0000	
0.351 (0 0 0 5 0)			
0.262 (0 0 0 5 2)			
0.387 (0 0 0 5 4)			
277.3376	277.3370	0.0006	
0.300 (0 0 0 5 2)			

0.590 (0 0 0 5 4)

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
210.2173	210.2170	0.0003	
0.436 (0 0 0 5 1)			
0.547 (0 0 0 5 3)			
263.7389	263.7391	-0.0002	
0.542 (0 0 0 5 1)			
0.366 (0 0 0 5 3)			
296.6776	296.6778	-0.0002	
0.891 (0 0 0 5 5)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
227.9449	227.9452	-0.0003	
0.492 (0 0 0 6 0)			
0.464 (0 0 0 6 2)			
324.9179	324.9176	0.0003	
0.304 (0 0 0 6 0)			
0.562 (0 0 0 6 4)			
375.4308	375.4313	-0.0005	
0.411 (0 0 0 6 2)			
0.317 (0 0 0 6 4)			
416.8463	416.8471	-0.0008	
0.906 (0 0 0 6 6)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
281.5945	281.5942	0.0003	
0.338 (0 0 0 6 1)			
0.610 (0 0 0 6 3)			
356.5151	356.5157	-0.0006	
0.536 (0 0 0 6 1)			
0.320 (0 0 0 6 5)			
391.8876	391.8869	0.0007	
0.628 (0 0 0 6 5)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
281.6023	281.6019	0.0004	
0.744 (0 0 0 6 2)			
0.251 (0 0 0 6 4)			
359.3662	359.3654	0.0008	
0.677 (0 0 0 6 4)			
416.5757	416.5766	-0.0009	
0.922 (0 0 0 6 6)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
227.9450	227.9453	-0.0003	
0.817 (0 0 0 6 1)			

	325.1463	325.1459	0.0004
0.639 (0 0 0 6 3)			
	387.8848	387.8836	0.0012
0.801 (0 0 0 6 5)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	362.3528	362.3524	0.0004
0.657 (0 0 0 7 2)			
0.327 (0 0 0 7 4)			
	458.6686	458.6682	0.0004
0.314 (0 0 0 7 2)			
0.481 (0 0 0 7 4)			
	524.3446	524.3434	0.0012
0.778 (0 0 0 7 6)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	298.9696	298.9700	-0.0004
0.778 (0 0 0 7 1)			
	415.5219	415.5216	0.0003
0.488 (0 0 0 7 3)			
0.315 (0 0 0 7 5)			
	493.3685	493.3676	0.0009
0.295 (0 0 0 7 3)			
0.600 (0 0 0 7 5)			
	556.9065	556.9082	-0.0017
0.919 (0 0 0 7 7)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	298.9696	298.9700	-0.0004
0.457 (0 0 0 7 0)			
0.478 (0 0 0 7 2)			
	415.4772	415.4769	0.0003
0.269 (0 0 0 7 0)			
0.614 (0 0 0 7 4)			
	487.2351	487.2366	-0.0015
0.401 (0 0 0 7 2)			
	526.6533	526.6525	0.0008
0.677 (0 0 0 7 6)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	362.3515	362.3511	0.0004
0.272 (0 0 0 7 1)			
0.628 (0 0 0 7 3)			
	457.8796	457.8799	-0.0003
0.441 (0 0 0 7 1)			
0.513 (0 0 0 7 5)			
	505.7564	505.7571	-0.0007
0.284 (0 0 0 7 1)			

0.340	(0 0 0 7 3)			
0.314	(0 0 0 7 5)			
		557.0299	557.0315	-0.0016
0.913	(0 0 0 7 7)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	379.4073	379.4078	-0.0005
0.428 (0 0 0 8 0)			
0.484 (0 0 0 8 2)			
	515.2886	515.2883	0.0003
0.597 (0 0 0 8 4)			
	608.5652	608.5665	-0.0013
0.296 (0 0 0 8 2)			
0.437 (0 0 0 8 6)			
	655.1943	655.1948	-0.0005
0.307 (0 0 0 8 4)			
0.341 (0 0 0 8 6)			
	716.9203	716.9226	-0.0023
0.915 (0 0 0 8 8)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	452.4943	452.4940	0.0003
0.622 (0 0 0 8 3)			
	567.6967	567.6968	-0.0001
0.356 (0 0 0 8 1)			
0.555 (0 0 0 8 5)			
	635.4082	635.4104	-0.0022
0.394 (0 0 0 8 1)			
0.320 (0 0 0 8 3)			
	681.6867	681.6857	0.0010
0.715 (0 0 0 8 7)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	452.4946	452.4942	0.0004
0.582 (0 0 0 8 2)			
0.383 (0 0 0 8 4)			
	567.8816	567.8815	0.0001
0.349 (0 0 0 8 2)			
0.303 (0 0 0 8 4)			
0.340 (0 0 0 8 6)			
	646.4593	646.4583	0.0010
0.307 (0 0 0 8 4)			
0.552 (0 0 0 8 6)			
	716.8650	716.8673	-0.0023
0.918 (0 0 0 8 8)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	379.4073	379.4078	-0.0005

0.743	(0 0 0 8 1)	515.2971	515.2968	0.0003
0.363	(0 0 0 8 3)			
0.407	(0 0 0 8 5)	610.7241	610.7239	0.0002
0.366	(0 0 0 8 3)			
0.378	(0 0 0 8 5)	680.4646	680.4634	0.0012
0.768	(0 0 0 8 7)			

SYMMETRY A1

	EIGENSTATE	Eexp	Ecalc	Residual
		552.0139	552.0136	0.0003
0.520	(0 0 0 9 2)			
0.421	(0 0 0 9 4)	686.5293	686.5293	0.0000
0.361	(0 0 0 9 2)			
0.433	(0 0 0 9 6)	781.2679	781.2678	0.0001
0.371	(0 0 0 9 4)			
0.315	(0 0 0 9 6)	856.1456	856.1445	0.0011
0.763	(0 0 0 9 8)			

SYMMETRY A2

	EIGENSTATE	Eexp	Ecalc	Residual
		469.2461	469.2467	-0.0006
0.713	(0 0 0 9 1)			
0.255	(0 0 0 9 3)	624.4145	624.4142	0.0003
0.267	(0 0 0 9 3)			
0.463	(0 0 0 9 5)	738.4675	738.4677	-0.0002
0.389	(0 0 0 9 3)			
0.341	(0 0 0 9 7)	818.6985	818.6974	0.0011
0.306	(0 0 0 9 5)			
0.525	(0 0 0 9 7)	896.1713	896.1737	-0.0024
0.916	(0 0 0 9 9)			

SYMMETRY B1

	EIGENSTATE	Eexp	Ecalc	Residual
		469.2461	469.2467	-0.0006
0.405	(0 0 0 9 0)			
0.486	(0 0 0 9 2)	624.4128	624.4126	0.0002
0.548	(0 0 0 9 4)	737.8607	737.8615	-0.0008
0.480	(0 0 0 9 6)	801.2849	801.2873	-0.0024
0.309	(0 0 0 9 2)			

0.279 (0 0 0 9 4)	856.7557	856.7547	0.0010
0.737 (0 0 0 9 8)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
552.0139	552.0135	0.0004	
0.604 (0 0 0 9 3)	686.4885	686.4886	-0.0001
0.295 (0 0 0 9 1)			
0.503 (0 0 0 9 5)	776.3768	776.3790	-0.0022
0.412 (0 0 0 9 1)			
0.354 (0 0 0 9 7)	824.2715	824.2715	0.0000
0.295 (0 0 0 9 5)			
0.384 (0 0 0 9 7)	896.1960	896.1984	-0.0024
0.915 (0 0 0 9 9)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
568.4725	568.4730	-0.0005	
0.385 (0 0 0 10 0)			
0.485 (0 0 0 10 2)	742.8526	742.8525	0.0001
0.488 (0 0 0 10 4)			
0.278 (0 0 0 10 6)	875.6318	875.6323	-0.0005
0.408 (0 0 0 10 6)	960.9002	960.9027	-0.0025
0.334 (0 0 0 10 2)			
0.283 (0 0 0 10 8)	1013.3421	1013.3416	0.0005
0.293 (0 0 0 10 6)			
0.427 (0 0 0 10 8)	1094.5218	1094.5237	-0.0019
0.913 (0 0 0 10 10)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
660.8967	660.8963	0.0004	
0.581 (0 0 0 10 3)	814.4569	814.4571	-0.0002
0.252 (0 0 0 10 1)			
0.416 (0 0 0 10 5)			
0.262 (0 0 0 10 7)	925.4386	925.4399	-0.0013
0.360 (0 0 0 10 1)			
0.406 (0 0 0 10 7)	985.3515	985.3533	-0.0018
0.251 (0 0 0 10 3)			

0.266 (0 0 0 10 5)	1051.5043	1051.5032	0.0011
0.748 (0 0 0 10 9)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
660.8967	660.8964	0.0003	
0.468 (0 0 0 10 2)			
0.445 (0 0 0 10 4)			
814.4658	814.4660	-0.0002	
0.360 (0 0 0 10 2)			
0.474 (0 0 0 10 6)			
927.1022	927.1026	-0.0004	
0.374 (0 0 0 10 4)			
0.330 (0 0 0 10 8)			
1010.1115	1010.1104	0.0011	
0.302 (0 0 0 10 6)			
0.510 (0 0 0 10 8)			
1094.5108	1094.5126	-0.0018	
0.913 (0 0 0 10 10)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
568.4725	568.4730	-0.0005	
0.686 (0 0 0 10 1)			
0.271 (0 0 0 10 3)			
742.8529	742.8528	0.0001	
0.488 (0 0 0 10 5)			
875.7862	875.7867	-0.0005	
0.377 (0 0 0 10 3)			
0.427 (0 0 0 10 7)			
970.3139	970.3137	0.0002	
0.360 (0 0 0 10 5)			
0.278 (0 0 0 10 7)			
1051.2106	1051.2094	0.0012	
0.760 (0 0 0 10 9)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
779.1273	779.1269	0.0004	
0.424 (0 0 0 11 2)			
0.459 (0 0 0 11 4)			
951.6482	951.6486	-0.0004	
0.352 (0 0 0 11 2)			
0.474 (0 0 0 11 6)			
1082.8075	1082.8080	-0.0005	
0.334 (0 0 0 11 4)			
0.406 (0 0 0 11 8)			
1177.9113	1177.9107	0.0006	
0.348 (0 0 0 11 6)			
0.256 (0 0 0 11 8)			
1265.4171	1265.4157	0.0014	

0.756 (0 0 0 11 10)

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
677.0716	677.0719	-0.0003	
0.663 (0 0 0 11 1)			
0.284 (0 0 0 11 3)			
870.5962	870.5963	-0.0001	
0.492 (0 0 0 11 5)			
1022.3647	1022.3652	-0.0005	
0.347 (0 0 0 11 3)			
0.450 (0 0 0 11 7)			
1133.6702	1133.6704	-0.0002	
0.346 (0 0 0 11 5)			
0.315 (0 0 0 11 9)			
1220.6590	1220.6580	0.0010	
0.299 (0 0 0 11 7)			
0.502 (0 0 0 11 9)			
1311.5438	1311.5446	-0.0008	
0.910 (0 0 0 11 11)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
677.0716	677.0719	-0.0003	
0.368 (0 0 0 11 0)			
0.483 (0 0 0 11 2)			
870.5961	870.5962	-0.0001	
0.427 (0 0 0 11 4)			
0.328 (0 0 0 11 6)			
1022.3267	1022.3272	-0.0005	
0.298 (0 0 0 11 6)			
0.286 (0 0 0 11 8)			
1129.7641	1129.7654	-0.0013	
0.283 (0 0 0 11 2)			
0.337 (0 0 0 11 8)			
1188.2356	1188.2363	-0.0007	
0.271 (0 0 0 11 6)			
1265.5557	1265.5543	0.0014	
0.751 (0 0 0 11 10)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
779.1273	779.1269	0.0004	
0.555 (0 0 0 11 3)			
0.265 (0 0 0 11 5)			
951.6463	951.6467	-0.0004	
0.325 (0 0 0 11 5)			
0.331 (0 0 0 11 7)			
1082.3184	1082.3189	-0.0005	
0.302 (0 0 0 11 1)			
0.329 (0 0 0 11 7)			
1162.1390	1162.1410	-0.0020	

0.311 (0 0 0 11 1)			
0.277 (0 0 0 11 3)			
	1222.3933	1222.3925	0.0008
0.293 (0 0 0 11 7)			
0.457 (0 0 0 11 9)			
	1311.5489	1311.5496	-0.0007
0.909 (0 0 0 11 11)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	795.0270	795.0270	0.0000
0.354 (0 0 0 12 0)			
0.479 (0 0 0 12 2)			
	1007.6266	1007.6269	-0.0003
0.370 (0 0 0 12 4)			
0.364 (0 0 0 12 6)			
	1178.0946	1178.0950	-0.0004
0.354 (0 0 0 12 8)			
	1306.0223	1306.0222	0.0001
0.267 (0 0 0 12 8)			
	1380.5115	1380.5121	-0.0006
	1451.1035	1451.1029	0.0006
0.295 (0 0 0 12 8)			
0.473 (0 0 0 12 10)			
	1546.9158	1546.9153	0.0005
0.905 (0 0 0 12 12)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	906.6886	906.6880	0.0006
0.529 (0 0 0 12 3)			
0.292 (0 0 0 12 5)			
	1098.0552	1098.0559	-0.0007
0.378 (0 0 0 12 7)			
	1247.6784	1247.6785	-0.0001
0.258 (0 0 0 12 1)			
0.293 (0 0 0 12 9)			
	1350.1910	1350.1915	-0.0005
0.340 (0 0 0 12 1)			
0.277 (0 0 0 12 9)			
	1410.5440	1410.5436	0.0004
0.286 (0 0 0 12 7)			
	1498.5401	1498.5385	0.0016
0.749 (0 0 0 12 11)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	906.6886	906.6880	0.0006
0.387 (0 0 0 12 2)			
0.465 (0 0 0 12 4)			
	1098.0557	1098.0563	-0.0006
0.341 (0 0 0 12 2)			

0.447 (0 0 0 12 6)	1247.8137	1247.8140	-0.0003
0.275 (0 0 0 12 4)			
0.411 (0 0 0 12 8)	1358.1292	1358.1289	0.0003
0.319 (0 0 0 12 6)			
0.302 (0 0 0 12 10)	1450.2211	1450.2204	0.0007
0.298 (0 0 0 12 8)			
0.495 (0 0 0 12 10)	1546.9135	1546.9129	0.0006
0.905 (0 0 0 12 12)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
795.0270	795.0270	0.0000	
0.642 (0 0 0 12 1)			
0.293 (0 0 0 12 3)	1007.6266	1007.6269	-0.0003
0.481 (0 0 0 12 5)	1178.1039	1178.1044	-0.0005
0.310 (0 0 0 12 3)			
0.423 (0 0 0 12 7)	1307.3605	1307.3606	-0.0001
0.283 (0 0 0 12 5)			
0.380 (0 0 0 12 9)	1404.1079	1404.1071	0.0008
0.338 (0 0 0 12 7)	1498.4754	1498.4738	0.0016
0.751 (0 0 0 12 11)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
1043.5618	1043.5609	0.0009	
0.355 (0 0 0 13 2)			
0.467 (0 0 0 13 4)	1253.6688	1253.6699	-0.0011
0.328 (0 0 0 13 2)			
0.404 (0 0 0 13 6)	1421.9064	1421.9064	0.0000
0.362 (0 0 0 13 8)	1549.2697	1549.2695	0.0002
0.262 (0 0 0 13 4)			
0.355 (0 0 0 13 10)	1648.9112	1648.9105	0.0007
0.331 (0 0 0 13 8)	1750.0643	1750.0627	0.0016
0.745 (0 0 0 13 12)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
922.3209	922.3205	0.0004	

0.623 (0 0 0 13 1)			
0.301 (0 0 0 13 3)			
	1153.9248	1153.9254	-0.0006
0.460 (0 0 0 13 5)			
	1342.9690	1342.9697	-0.0007
0.273 (0 0 0 13 3)			
0.367 (0 0 0 13 7)			
	1490.5152	1490.5149	0.0003
0.260 (0 0 0 13 3)			
0.371 (0 0 0 13 9)			
	1600.5002	1600.4997	0.0005
0.299 (0 0 0 13 7)			
0.294 (0 0 0 13 11)			
	1698.5980	1698.5983	-0.0003
0.298 (0 0 0 13 9)			
0.487 (0 0 0 13 11)			
	1800.2511	1800.2496	0.0015
0.899 (0 0 0 13 13)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	922.3209	922.3205	0.0004
0.341 (0 0 0 13 0)			
0.474 (0 0 0 13 2)			
	1153.9248	1153.9254	-0.0006
0.319 (0 0 0 13 4)			
0.388 (0 0 0 13 6)			
	1342.9667	1342.9673	-0.0006
0.391 (0 0 0 13 8)			
	1490.0983	1490.0974	0.0009
0.287 (0 0 0 13 10)			
	1586.4081	1586.4072	0.0009
0.285 (0 0 0 13 2)			
	1652.5839	1652.5832	0.0007
0.300 (0 0 0 13 8)			
	1750.0945	1750.0930	0.0015
0.744 (0 0 0 13 12)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	1043.5618	1043.5609	0.0009
0.503 (0 0 0 13 3)			
0.314 (0 0 0 13 5)			
	1253.6687	1253.6698	-0.0011
0.404 (0 0 0 13 7)			
	1421.8697	1421.8695	0.0002
0.257 (0 0 0 13 5)			
0.357 (0 0 0 13 9)			
	1546.0584	1546.0571	0.0013
0.312 (0 0 0 13 1)			
	1616.7080	1616.7074	0.0006
	1699.0317	1699.0320	-0.0003

0.296 (0 0 0 13 9)			
0.477 (0 0 0 13 11)			
	1800.2522	1800.2507	0.0015
0.899 (0 0 0 13 13)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	1058.9341	1058.9333	0.0008
0.329 (0 0 0 14 0)			
0.469 (0 0 0 14 2)			
	1309.4693	1309.4703	-0.0010
0.274 (0 0 0 14 4)			
0.402 (0 0 0 14 6)			
	1516.9375	1516.9383	-0.0008
0.254 (0 0 0 14 4)			
0.398 (0 0 0 14 8)			
	1682.6051	1682.6036	0.0015
0.267 (0 0 0 14 6)			
0.346 (0 0 0 14 10)			
	1801.6504	1801.6478	0.0026
0.266 (0 0 0 14 2)			
	1871.5268	1871.5259	0.0009
	1965.7326	1965.7348	-0.0022
0.298 (0 0 0 14 10)			
0.473 (0 0 0 14 12)			
	2071.1811	2071.1805	0.0006
0.892 (0 0 0 14 14)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	1189.7266	1189.7253	0.0013
0.479 (0 0 0 14 3)			
0.331 (0 0 0 14 5)			
	1418.4664	1418.4681	-0.0017
0.411 (0 0 0 14 7)			
	1605.0037	1605.0032	0.0005
0.275 (0 0 0 14 5)			
0.379 (0 0 0 14 9)			
	1749.0594	1749.0571	0.0023
0.269 (0 0 0 14 1)			
0.271 (0 0 0 14 11)			
	1838.6475	1838.6459	0.0016
0.250 (0 0 0 14 1)			
	1914.2137	1914.2134	0.0003
0.310 (0 0 0 14 9)			
	2019.8586	2019.8573	0.0013
0.735 (0 0 0 14 13)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1189.7266	1189.7253	0.0013
0.328 (0 0 0 14 2)			

0.464 (0 0 0 14 4)	1418.4665	1418.4681	-0.0016
0.314 (0 0 0 14 2)			
0.355 (0 0 0 14 6)			
0.285 (0 0 0 14 8)	1605.0137	1605.0133	0.0004
0.286 (0 0 0 14 8)	1750.1937	1750.1932	0.0005
0.270 (0 0 0 14 4)			
0.334 (0 0 0 14 10)	1860.8359	1860.8357	0.0002
0.286 (0 0 0 14 8)			
0.290 (0 0 0 14 12)	1965.5238	1965.5261	-0.0023
0.299 (0 0 0 14 10)			
0.477 (0 0 0 14 12)	2071.1822	2071.1799	0.0023
0.892 (0 0 0 14 14)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	1058.9341	1058.9333	0.0008
0.605 (0 0 0 14 1)			
0.307 (0 0 0 14 3)	1309.4693	1309.4703	-0.0010
0.435 (0 0 0 14 5)			
0.254 (0 0 0 14 7)	1516.9381	1516.9389	-0.0008
0.299 (0 0 0 14 7)			
0.281 (0 0 0 14 9)	1682.7300	1682.7291	0.0009
0.263 (0 0 0 14 3)			
0.305 (0 0 0 14 9)	1808.4391	1808.4392	-0.0001
0.262 (0 0 0 14 5)			
0.334 (0 0 0 14 11)	1912.2568	1912.2567	0.0001
0.327 (0 0 0 14 9)	2019.8444	2019.8431	0.0013
0.736 (0 0 0 14 13)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	1345.1614	1345.1594	0.0020
0.304 (0 0 0 15 2)			
0.459 (0 0 0 15 4)	1592.4251	1592.4273	-0.0022
0.301 (0 0 0 15 2)			
0.305 (0 0 0 15 6)			
0.317 (0 0 0 15 8)	1797.1045	1797.1038	0.0007
0.302 (0 0 0 15 10)			

	1960.2477	1960.2468	0.0009
0.257 (0 0 0 15 4)			
0.258 (0 0 0 15 10)			
	2084.8553	2084.8571	-0.0018
0.255 (0 0 0 15 6)			
0.319 (0 0 0 15 12)			
	2193.9945	2193.9958	-0.0013
0.324 (0 0 0 15 10)			
	2307.4672	2307.4655	0.0017
0.725 (0 0 0 15 14)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	1204.8460	1204.8449	0.0011
0.590 (0 0 0 15 1)			
0.311 (0 0 0 15 3)			
	1474.2372	1474.2385	-0.0013
0.407 (0 0 0 15 5)			
0.281 (0 0 0 15 7)			
	1699.9886	1699.9896	-0.0010
0.321 (0 0 0 15 9)			
	1883.8520	1883.8504	0.0016
0.256 (0 0 0 15 3)			
0.260 (0 0 0 15 11)			
	2026.6264	2026.6272	-0.0008
0.259 (0 0 0 15 5)			
0.302 (0 0 0 15 11)			
	2139.1772	2139.1773	-0.0001
0.277 (0 0 0 15 9)			
0.291 (0 0 0 15 13)			
	2250.6858	2250.6880	-0.0022
0.302 (0 0 0 15 11)			
0.464 (0 0 0 15 13)			
	0.0000	2359.3302	0.0000
0.883 (0 0 0 15 15)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1204.8460	1204.8449	0.0011
0.319 (0 0 0 15 0)			
0.464 (0 0 0 15 2)			
	1474.2372	1474.2385	-0.0013
0.408 (0 0 0 15 6)			
	1699.9884	1699.9895	-0.0011
0.264 (0 0 0 15 4)			
0.382 (0 0 0 15 8)			
	1883.8150	1883.8130	0.0020
0.263 (0 0 0 15 6)			
0.355 (0 0 0 15 10)			
	2023.8717	2023.8686	0.0031
	2107.6049	2107.6044	0.0005
	2194.9891	2194.9900	-0.0009

0.316 (0 0 0 15 10)	2307.4739	2307.4722	0.0017
0.724 (0 0 0 15 14)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
1345.1614	1345.1594	0.0020	
0.456 (0 0 0 15 3)			
0.344 (0 0 0 15 5)			
1592.4250	1592.4273	-0.0023	
0.404 (0 0 0 15 7)			
1797.1018	1797.1010	0.0008	
0.273 (0 0 0 15 5)			
0.367 (0 0 0 15 9)			
1959.8719	1959.8693	0.0026	
0.252 (0 0 0 15 7)			
0.327 (0 0 0 15 11)			
2072.2125	2072.2098	0.0027	
0.290 (0 0 0 15 1)			
2145.5971	2145.5964	0.0007	
2250.7852	2250.7874	-0.0022	
0.301 (0 0 0 15 11)			
0.462 (0 0 0 15 13)			
2359.3282	2359.3305	-0.0023	
0.883 (0 0 0 15 15)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
1360.0338	1360.0334	0.0004	
0.310 (0 0 0 16 0)			
0.459 (0 0 0 16 2)			
1648.2045	1648.2055	-0.0010	
0.407 (0 0 0 16 6)			
1892.0956	1892.0965	-0.0009	
0.266 (0 0 0 16 4)			
0.352 (0 0 0 16 8)			
2093.8133	2093.8108	0.0025	
0.325 (0 0 0 16 10)			
2253.1372	2253.1351	0.0021	
0.302 (0 0 0 16 12)			
2357.7159	2357.7163	-0.0004	
2439.0694	2439.0697	-0.0003	
0.270 (0 0 0 16 14)			
2553.7880	2553.7920	-0.0040	
0.304 (0 0 0 16 12)			
0.446 (0 0 0 16 14)			
0.0000	2664.3165	0.0000	
0.873 (0 0 0 16 16)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
1509.8427	1509.8401	0.0026	

0.435	(0 0 0 16 3)			
0.354	(0 0 0 16 5)			
		1775.5189	1775.5217	-0.0028
0.387	(0 0 0 16 7)			
		1998.1538	1998.1526	0.0012
0.259	(0 0 0 16 5)			
0.330	(0 0 0 16 9)			
		2179.0142	2179.0114	0.0028
0.326	(0 0 0 16 11)			
		2313.6934	2313.6901	0.0033
0.281	(0 0 0 16 1)			
		2394.2291	2394.2295	-0.0004
		2494.3839	2494.3808	0.0031
0.318	(0 0 0 16 11)			
		2612.5856	2612.5891	-0.0035
0.711	(0 0 0 16 15)			

SYMMETRY B1

	EIGENSTATE	Eexp	Ecalc	Residual
		1509.8429	1509.8401	0.0028
0.283	(0 0 0 16 2)			
0.452	(0 0 0 16 4)			
		1775.5188	1775.5217	-0.0029
0.288	(0 0 0 16 2)			
0.258	(0 0 0 16 6)			
0.340	(0 0 0 16 8)			
		1998.1546	1998.1534	0.0012
0.334	(0 0 0 16 10)			
		2179.1355	2179.1345	0.0010
0.263	(0 0 0 16 12)			
		2319.6719	2319.6770	-0.0051
0.278	(0 0 0 16 12)			
		2435.5106	2435.5117	-0.0011
0.271	(0 0 0 16 10)			
0.295	(0 0 0 16 14)			
		2553.7408	2553.7449	-0.0041
0.305	(0 0 0 16 12)			
0.447	(0 0 0 16 14)			
		2664.3152	2664.3164	-0.0012
0.873	(0 0 0 16 16)			

SYMMETRY B2

	EIGENSTATE	Eexp	Ecalc	Residual
		1360.0338	1360.0334	0.0004
0.576	(0 0 0 16 1)			
0.315	(0 0 0 16 3)			
		1648.2045	1648.2055	-0.0010
0.379	(0 0 0 16 5)			
0.303	(0 0 0 16 7)			
		1892.0954	1892.0966	-0.0012
0.345	(0 0 0 16 9)			
		2093.8243	2093.8219	0.0024

0.309	(0 0 0 16 11)	2254.1518	2254.1528	-0.0010
		2378.5653	2378.5676	-0.0023
0.310	(0 0 0 16 13)	2493.8937	2493.8909	0.0028
0.322	(0 0 0 16 11)	2612.5824	2612.5858	-0.0034
0.711	(0 0 0 16 15)			

SYMMETRY A1

	EIGENSTATE	Eexp	Ecalc	Residual
		1683.7467	1683.7427	0.0040
0.265	(0 0 0 17 2)			
0.444	(0 0 0 17 4)			
		1967.7198	1967.7235	-0.0037
0.275	(0 0 0 17 2)			
0.353	(0 0 0 17 8)			
		2208.1370	2208.1360	0.0010
0.345	(0 0 0 17 10)			
		2406.7409	2406.7395	0.0014
0.305	(0 0 0 17 12)			
		2564.1843	2564.1929	-0.0086
		2689.6345	2689.6395	-0.0050
0.305	(0 0 0 17 14)			
		2811.6606	2811.6549	0.0057
0.320	(0 0 0 17 12)			
		0.0000	2934.8338	0.0000
0.695	(0 0 0 17 16)			

SYMMETRY A2

	EIGENSTATE	Eexp	Ecalc	Residual
		1524.4752	1524.4756	-0.0004
0.563	(0 0 0 17 1)			
0.317	(0 0 0 17 3)			
		1831.3425	1831.3447	-0.0022
0.351	(0 0 0 17 5)			
0.320	(0 0 0 17 7)			
		2093.2302	2093.2316	-0.0014
0.355	(0 0 0 17 9)			
		2312.6163	2312.6125	0.0038
0.330	(0 0 0 17 11)			
		2490.5151	2490.5156	-0.0005
0.260	(0 0 0 17 13)			
		2629.2850	2629.2913	-0.0063
0.259	(0 0 0 17 13)			
		2749.7398	2749.7343	0.0055
0.266	(0 0 0 17 11)			
0.303	(0 0 0 17 15)			
		2874.3293	2874.3384	-0.0091
0.308	(0 0 0 17 13)			
0.426	(0 0 0 17 15)			
		0.0000	2985.7757	0.0000

0.860 (0 0 0 17 17)

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
1524.4752	1524.4756	-0.0004	
0.302 (0 0 0 17 0)			
0.454 (0 0 0 17 2)			
1831.3433	1831.3447	-0.0014	
0.402 (0 0 0 17 6)			
2093.2300	2093.2317	-0.0017	
0.262 (0 0 0 17 4)			
0.313 (0 0 0 17 8)			
0.251 (0 0 0 17 10)			
2312.6130	2312.6097	0.0033	
0.271 (0 0 0 17 10)			
2490.1580	2490.1577	0.0003	
0.295 (0 0 0 17 12)			
2617.7428	2617.7439	-0.0011	
2699.4367	2699.4392	-0.0025	
2811.8977	2811.8917	0.0060	
0.318 (0 0 0 17 12)			
2934.8467	2934.8354	0.0113	
0.695 (0 0 0 17 16)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
1683.7466	1683.7427	0.0039	
0.415 (0 0 0 17 3)			
0.361 (0 0 0 17 5)			
1967.7197	1967.7235	-0.0038	
0.364 (0 0 0 17 7)			
2208.1378	2208.1355	0.0023	
0.279 (0 0 0 17 9)			
2406.7020	2406.6982	0.0038	
0.282 (0 0 0 17 11)			
2561.7083	2561.7050	0.0033	
0.273 (0 0 0 17 13)			
2658.7846	2658.7864	-0.0018	
2751.6002	2751.5939	0.0063	
0.250 (0 0 0 17 11)			
0.289 (0 0 0 17 15)			
2874.3517	2874.3607	-0.0090	
0.308 (0 0 0 17 13)			
0.425 (0 0 0 17 15)			
2985.7762	2985.7757	0.0005	
0.860 (0 0 0 17 17)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
1698.1446	1698.1467	-0.0021	
0.295 (0 0 0 18 0)			
0.449 (0 0 0 18 2)			

	2023.6257	2023.6282	-0.0025
0.393 (0 0 0 18 6)	2303.3616	2303.3645	-0.0029
0.255 (0 0 0 18 4)			
0.271 (0 0 0 18 8)			
0.280 (0 0 0 18 10)			
	2540.1995	2540.1953	0.0042
0.264 (0 0 0 18 12)			
	2735.3660	2735.3671	-0.0011
	2884.7108	2884.7125	-0.0017
	2976.4822	2976.4861	-0.0039
	3082.5939	3082.5945	-0.0006
0.253 (0 0 0 18 12)			
0.305 (0 0 0 18 16)			
	0.0000	3212.0753	0.0000
0.311 (0 0 0 18 14)			
0.400 (0 0 0 18 16)			
	0.0000	3323.3420	0.0000
0.844 (0 0 0 18 18)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	1866.8408	0.0000
0.397 (0 0 0 18 3)			
0.366 (0 0 0 18 5)			
	2168.9974	2169.0031	-0.0057
0.338 (0 0 0 18 7)			
0.260 (0 0 0 18 9)			
	2427.0234	2427.0213	0.0021
0.280 (0 0 0 18 11)			
	2643.0020	2642.9959	0.0061
	2816.7062	2816.7034	0.0028
0.264 (0 0 0 18 13)			
	2935.7303	2935.7310	-0.0007
	3023.7163	3023.7116	0.0047
0.264 (0 0 0 18 15)			
	3147.0477	3147.0588	-0.0111
0.316 (0 0 0 18 13)			
0.251 (0 0 0 18 17)			
	0.0000	3273.8871	0.0000
0.675 (0 0 0 18 17)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1866.8458	1866.8408	0.0050
0.436 (0 0 0 18 4)			
	2168.9981	2169.0031	-0.0050
0.263 (0 0 0 18 2)			
0.358 (0 0 0 18 8)			
	2427.0241	2427.0219	0.0022
0.337 (0 0 0 18 10)			
	2643.0145	2643.0121	0.0024

0.315 (0 0 0 18 12)	2817.6608	2817.6719	-0.0111
0.253 (0 0 0 18 14)	2955.5056	2955.5177	-0.0121
	3081.6794	3081.6608	0.0186
0.261 (0 0 0 18 12)			
0.312 (0 0 0 18 16)	3212.0457	3212.0646	-0.0189
0.311 (0 0 0 18 14)			
0.400 (0 0 0 18 16)	0.0000	3323.3420	0.0000
0.844 (0 0 0 18 18)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
1698.1446	1698.1467	-0.0021	
0.551 (0 0 0 18 1)			
0.319 (0 0 0 18 3)	2023.6265	2023.6282	-0.0017
0.325 (0 0 0 18 5)			
0.332 (0 0 0 18 7)	2303.3623	2303.3643	-0.0020
0.351 (0 0 0 18 9)	2540.2003	2540.1948	0.0055
0.325 (0 0 0 18 11)	2735.4894	2735.4879	0.0015
0.295 (0 0 0 18 13)	2890.1707	2890.1818	-0.0111
	3018.0963	3018.0949	0.0014
0.305 (0 0 0 18 15)	3146.9607	3146.9457	0.0150
0.317 (0 0 0 18 13)			
0.252 (0 0 0 18 17)	3273.8946	3273.8863	0.0083
0.676 (0 0 0 18 17)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2059.1152	2059.1063	0.0089	
0.427 (0 0 0 19 4)			
0.257 (0 0 0 19 6)	2379.3216	2379.3290	-0.0074
0.253 (0 0 0 19 2)			
0.357 (0 0 0 19 8)	2654.7799	2654.7787	0.0012
0.315 (0 0 0 19 10)	2887.9230	2887.9203	0.0027
0.296 (0 0 0 19 12)	3079.7070	3079.7182	-0.0112
0.281 (0 0 0 19 14)	0.0000	3232.0626	0.0000
	0.0000	3363.8823	0.0000

0.306 (0 0 0 19 16)	0.0000	3499.3689	0.0000
0.312 (0 0 0 19 14)			
0.268 (0 0 0 19 18)	0.0000	3629.3951	0.0000
0.259 (0 0 0 19 16)			
0.653 (0 0 0 19 18)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
1881.0158	1881.0199	-0.0041	
0.540 (0 0 0 19 1)			
0.321 (0 0 0 19 3)	2225.0238	2225.0260	-0.0022
0.300 (0 0 0 19 5)			
0.340 (0 0 0 19 7)	2522.4579	2522.4618	-0.0039
0.339 (0 0 0 19 9)	2776.5451	2776.5385	0.0066
0.301 (0 0 0 19 11)	2988.9802	2988.9746	0.0056
0.294 (0 0 0 19 13)	3160.2907	3160.3079	-0.0172
	0.0000	3298.4272	0.0000
	0.0000	3431.0152	0.0000
0.254 (0 0 0 19 13)			
0.322 (0 0 0 19 17)	0.0000	3566.5721	0.0000
0.314 (0 0 0 19 15)			
0.370 (0 0 0 19 17)	0.0000	3676.6641	0.0000
0.824 (0 0 0 19 19)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
1881.0158	1881.0199	-0.0041	
0.288 (0 0 0 19 0)			
0.444 (0 0 0 19 2)	2225.0246	2225.0261	-0.0015
0.383 (0 0 0 19 6)	2522.4586	2522.4621	-0.0035
0.301 (0 0 0 19 10)	2776.5459	2776.5411	0.0048
0.292 (0 0 0 19 12)	2988.9378	2988.9383	-0.0005
	3157.9645	3157.9668	-0.0023
	3268.1516	3268.1460	0.0056
	0.0000	3366.8876	0.0000
0.283 (0 0 0 19 16)	0.0000	3499.4227	0.0000
0.312 (0 0 0 19 14)			
0.268 (0 0 0 19 18)			

	0.0000	3629.3955	0.0000
0.259 (0 0 0 19 16)			
0.653 (0 0 0 19 18)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	2059.1146	2059.1063	0.0083
0.381 (0 0 0 19 3)			
0.369 (0 0 0 19 5)			
	2379.3223	2379.3289	-0.0066
0.310 (0 0 0 19 7)			
0.280 (0 0 0 19 9)			
	2654.7806	2654.7775	0.0031
0.302 (0 0 0 19 11)			
	2887.9185	2887.9103	0.0082
0.272 (0 0 0 19 13)			
	3079.3512	3079.3487	0.0025
	3221.2386	3221.2346	0.0040
0.256 (0 0 0 19 1)			
	3311.9811	3311.9732	0.0079
	0.0000	3431.4718	0.0000
0.251 (0 0 0 19 13)			
0.319 (0 0 0 19 17)			
	0.0000	3566.5772	0.0000
0.313 (0 0 0 19 15)			
0.370 (0 0 0 19 17)			
	0.0000	3676.6641	0.0000
0.824 (0 0 0 19 19)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	2073.0610	2073.0666	-0.0056
0.282 (0 0 0 20 0)			
0.440 (0 0 0 20 2)			
	2435.5060	2435.5065	-0.0005
0.370 (0 0 0 20 6)			
	2750.4835	2750.4899	-0.0064
0.313 (0 0 0 20 10)			
	3021.6183	3021.6148	0.0035
0.305 (0 0 0 20 12)			
	0.0000	3250.9239	0.0000
0.272 (0 0 0 20 14)			
	0.0000	3438.1146	0.0000
	0.0000	3570.7568	0.0000
	0.0000	3666.0451	0.0000
	0.0000	3797.6684	0.0000
0.331 (0 0 0 20 18)			
	0.0000	3937.4349	0.0000
0.314 (0 0 0 20 16)			
0.336 (0 0 0 20 18)			
	0.0000	4045.4178	0.0000
0.799 (0 0 0 20 20)			

SYMMETRY A2				
EIGENSTATE		Eexp	Ecalc	Residual
		2260.5236	2260.5090	0.0146
0.365	(0 0 0 20 3)			
0.370	(0 0 0 20 5)			
		2598.6588	2598.6674	-0.0086
0.281	(0 0 0 20 7)			
0.296	(0 0 0 20 9)			
		2891.3712	2891.3689	0.0023
0.313	(0 0 0 20 11)			
		0.0000	3141.4232	0.0000
0.292	(0 0 0 20 13)			
		0.0000	3350.0052	0.0000
		0.0000	3513.0347	0.0000
		0.0000	3616.1107	0.0000
		0.0000	3728.3866	0.0000
0.297	(0 0 0 20 17)			
		0.0000	3868.6029	0.0000
0.306	(0 0 0 20 15)			
0.287	(0 0 0 20 19)			
		0.0000	4001.0378	0.0000
0.272	(0 0 0 20 17)			
0.628	(0 0 0 20 19)			

SYMMETRY B1				
EIGENSTATE		Eexp	Ecalc	Residual
		2260.5235	2260.5090	0.0145
0.418	(0 0 0 20 4)			
0.266	(0 0 0 20 6)			
		2598.6592	2598.6675	-0.0083
0.350	(0 0 0 20 8)			
		2891.3719	2891.3711	0.0008
0.285	(0 0 0 20 10)			
		3141.4349	3141.4331	0.0018
0.257	(0 0 0 20 12)			
		3350.1313	3350.1476	-0.0163
0.270	(0 0 0 20 14)			
		0.0000	3518.2377	0.0000
		0.0000	3658.0693	0.0000
		0.0000	3797.4487	0.0000
0.333	(0 0 0 20 18)			
		0.0000	3937.4324	0.0000
0.314	(0 0 0 20 16)			
0.336	(0 0 0 20 18)			
		0.0000	4045.4178	0.0000
0.799	(0 0 0 20 20)			

SYMMETRY B2				
EIGENSTATE		Eexp	Ecalc	Residual
		2073.0610	2073.0666	-0.0056
0.530	(0 0 0 20 1)			

0.322 (0 0 0 20 3)	2435.5068	2435.5065	0.0003
0.276 (0 0 0 20 5)			
0.345 (0 0 0 20 7)	2750.4842	2750.4892	-0.0050
0.319 (0 0 0 20 9)	3021.6191	3021.6098	0.0093
0.263 (0 0 0 20 11)	3250.9424	3250.9295	0.0129
0.263 (0 0 0 20 13)	0.0000	3439.0686	0.0000
0.265 (0 0 0 20 15)	0.0000	3589.8529	0.0000
	0.0000	3726.8542	0.0000
0.308 (0 0 0 20 17)	0.0000	3868.5774	0.0000
0.306 (0 0 0 20 15)			
0.287 (0 0 0 20 19)	0.0000	4001.0376	0.0000
0.272 (0 0 0 20 17)			
0.628 (0 0 0 20 19)			

POLYAD P = 1

	EIGENSTATE	Eexp	Ecalc	Residual
	1197.9671	1197.9630	0.0041	
1.000 (0 1 0 1 1)				

	EIGENSTATE	Eexp	Ecalc	Residual
	1196.4671	1196.4629	0.0042	
1.000 (0 1 0 1 0)				

	EIGENSTATE	Eexp	Ecalc	Residual
	1202.5198	1202.5160	0.0038	
1.000 (0 1 0 1 1)				

	EIGENSTATE	Eexp	Ecalc	Residual
	1220.8682	1220.8642	0.0040	
0.846 (0 1 0 2 0)	1242.6855	1242.6823	0.0032	
0.846 (0 1 0 2 2)				

	EIGENSTATE	Eexp	Ecalc	Residual
	1234.8380	1234.8342	0.0037	
1.000 (0 1 0 2 1)				

SYMMETRY B1			
EIGENSTATE	Eexp	Ecalc	Residual
1239.3239	1239.3209	0.0030	
1.000 (0 1 0 2 2)			

SYMMETRY B2			
EIGENSTATE	Eexp	Ecalc	Residual
1221.1956	1221.1919	0.0038	
1.000 (0 1 0 2 1)			

SYMMETRY A1			
EIGENSTATE	Eexp	Ecalc	Residual
1280.9878	1280.9848	0.0031	
1.000 (0 1 0 3 2)			

SYMMETRY A2			
EIGENSTATE	Eexp	Ecalc	Residual
1254.3133	1254.3094	0.0039	
0.964 (0 1 0 3 1)			
1301.4352	1301.4334	0.0018	
0.964 (0 1 0 3 3)			

SYMMETRY B1			
EIGENSTATE	Eexp	Ecalc	Residual
1254.2635	1254.2597	0.0038	
0.698 (0 1 0 3 0)			
0.302 (0 1 0 3 2)			
1292.5525	1292.5499	0.0027	
0.302 (0 1 0 3 0)			
0.698 (0 1 0 3 2)			

SYMMETRY B2			
EIGENSTATE	Eexp	Ecalc	Residual
1279.4408	1279.4378	0.0029	
0.842 (0 1 0 3 1)			
1303.5420	1303.5401	0.0019	
0.842 (0 1 0 3 3)			

SYMMETRY A1			
EIGENSTATE	Eexp	Ecalc	Residual
1296.8609	1296.8572	0.0037	
0.604 (0 1 0 4 0)			
0.388 (0 1 0 4 2)			
1356.6618	1356.6595	0.0023	
0.373 (0 1 0 4 0)			
0.508 (0 1 0 4 2)			
1385.4729	1385.4724	0.0005	
0.872 (0 1 0 4 4)			

SYMMETRY A2			
EIGENSTATE	Eexp	Ecalc	Residual
1333.1196	1333.1170	0.0025	

0.604	(0 1 0 4 1)			
0.396	(0 1 0 4 3)			
		1369.8660	1369.8639	0.0022
0.396	(0 1 0 4 1)			
0.604	(0 1 0 4 3)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1333.4555	1333.4531	0.0024
0.941 (0 1 0 4 2)			
	1384.3290	1384.3286	0.0004
0.941 (0 1 0 4 4)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	1296.8675	1296.8641	0.0034
0.914 (0 1 0 4 1)			
	1360.8360	1360.8343	0.0017
0.914 (0 1 0 4 3)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	1395.6779	1395.6757	0.0023
0.847 (0 1 0 5 2)			
	1460.8304	1460.8289	0.0015
0.847 (0 1 0 5 4)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	1348.7573	1348.7540	0.0033
0.864 (0 1 0 5 1)			
	1432.1291	1432.1274	0.0017
0.799 (0 1 0 5 3)			
	1487.9663	1487.9669	-0.0006
0.930 (0 1 0 5 5)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1348.7561	1348.7530	0.0031
0.541 (0 1 0 5 0)			
0.436 (0 1 0 5 2)			
	1430.8672	1430.8661	0.0011
0.354 (0 1 0 5 0)			
0.272 (0 1 0 5 2)			
0.375 (0 1 0 5 4)			
	1467.1894	1467.1890	0.0004
0.292 (0 1 0 5 2)			
0.602 (0 1 0 5 4)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	1395.6168	1395.6157	0.0011

0.442	(0 1 0 5 1)			
0.542	(0 1 0 5 3)			
		1452.4261	1452.4254	0.0007
0.538	(0 1 0 5 1)			
0.375	(0 1 0 5 3)			
		1488.5274	1488.5280	-0.0006
0.897	(0 1 0 5 5)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	1409.9606	1409.9577	0.0030
0.495 (0 1 0 6 0)			
0.463 (0 1 0 6 2)			
	1513.4604	1513.4594	0.0011
0.307 (0 1 0 6 0)			
0.554 (0 1 0 6 4)			
	1566.9438	1566.9446	-0.0009
0.407 (0 1 0 6 2)			
0.328 (0 1 0 6 4)			
	1612.4771	1612.4783	-0.0011
0.911 (0 1 0 6 6)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	1467.2762	1467.2747	0.0014
0.342 (0 1 0 6 1)			
0.607 (0 1 0 6 3)			
	1546.9138	1546.9134	0.0004
0.541 (0 1 0 6 1)			
0.306 (0 1 0 6 5)			
	1585.0310	1585.0308	0.0002
0.644 (0 1 0 6 5)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1467.2855	1467.2849	0.0006
0.749 (0 1 0 6 2)			
	1550.3079	1550.3076	0.0003
0.684 (0 1 0 6 4)			
	1612.2181	1612.2193	-0.0012
0.925 (0 1 0 6 6)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	1409.9602	1409.9578	0.0024
0.819 (0 1 0 6 1)			
	1513.7461	1513.7465	-0.0005
0.646 (0 1 0 6 3)			
	1581.0428	1581.0432	-0.0004
0.807 (0 1 0 6 5)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
1548.1932	1548.1927	0.0005	
0.662 (0 1 0 7 2)			
0.323 (0 1 0 7 4)			
1650.9000	1650.8996	0.0005	
0.311 (0 1 0 7 2)			
0.490 (0 1 0 7 4)			
1721.5051	1721.5053	-0.0002	
0.786 (0 1 0 7 6)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
1480.4680	1480.4654	0.0026	
0.780 (0 1 0 7 1)			
1604.9129	1604.9124	0.0005	
0.496 (0 1 0 7 3)			
0.309 (0 1 0 7 5)			
1688.0234	1688.0244	-0.0010	
0.289 (0 1 0 7 3)			
0.609 (0 1 0 7 5)			
1756.8691	1756.8700	-0.0009	
0.923 (0 1 0 7 7)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
1480.4673	1480.4653	0.0020	
0.459 (0 1 0 7 0)			
0.477 (0 1 0 7 2)			
1604.8527	1604.8537	-0.0010	
0.271 (0 1 0 7 0)			
0.612 (0 1 0 7 4)			
1680.8121	1680.8144	-0.0023	
0.405 (0 1 0 7 2)			
1723.7440	1723.7452	-0.0012	
0.693 (0 1 0 7 6)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
1548.1909	1548.1909	0.0000	
0.276 (0 1 0 7 1)			
0.627 (0 1 0 7 3)			
1649.9135	1649.9151	-0.0016	
0.449 (0 1 0 7 1)			
0.503 (0 1 0 7 5)			
1700.6221	1700.6238	-0.0017	
0.273 (0 1 0 7 1)			
0.338 (0 1 0 7 3)			
0.329 (0 1 0 7 5)			
1756.9847	1756.9857	-0.0009	
0.917 (0 1 0 7 7)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
1560.2689	1560.2668	0.0021	
0.430 (0 1 0 8 0)			
0.484 (0 1 0 8 2)			
1705.3603	1705.3602	0.0002	
0.598 (0 1 0 8 4)			
1804.3489	1804.3505	-0.0016	
0.306 (0 1 0 8 2)			
0.424 (0 1 0 8 6)			
1854.0113	1854.0131	-0.0018	
0.305 (0 1 0 8 4)			
0.361 (0 1 0 8 6)			
1921.6838	1921.6836	0.0001	
0.919 (0 1 0 8 8)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
1638.3774	1638.3764	0.0010	
0.623 (0 1 0 8 3)			
1761.1356	1761.1353	0.0003	
0.362 (0 1 0 8 1)			
0.553 (0 1 0 8 5)			
1832.5187	1832.5194	-0.0007	
0.388 (0 1 0 8 1)			
0.325 (0 1 0 8 3)			
1883.3221	1883.3223	-0.0002	
0.729 (0 1 0 8 7)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
1638.3756	1638.3767	-0.0011	
0.587 (0 1 0 8 2)			
0.379 (0 1 0 8 4)			
1761.3747	1761.3763	-0.0016	
0.347 (0 1 0 8 2)			
0.313 (0 1 0 8 4)			
0.332 (0 1 0 8 6)			
1845.3375	1845.3389	-0.0014	
0.301 (0 1 0 8 4)			
0.564 (0 1 0 8 6)			
1921.6327	1921.6327	0.0000	
0.921 (0 1 0 8 8)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
1560.2683	1560.2668	0.0015	
0.746 (0 1 0 8 1)			
1705.3701	1705.3718	-0.0017	
0.371 (0 1 0 8 3)			
0.401 (0 1 0 8 5)			
1807.0130	1807.0149	-0.0019	
0.362 (0 1 0 8 3)			

0.390 (0 1 0 8 5)	1882.1650	1882.1663	-0.0013
0.776 (0 1 0 8 7)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
1737.8255	1737.8252	0.0004	
0.525 (0 1 0 9 2)			
0.417 (0 1 0 9 4)			
1881.2021	1881.2009	0.0012	
0.360 (0 1 0 9 2)			
0.427 (0 1 0 9 6)			
1982.0457	1982.0457	0.0000	
0.368 (0 1 0 9 4)			
0.329 (0 1 0 9 6)			
2062.8850	2062.8851	-0.0001	
0.772 (0 1 0 9 8)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
1649.3524	1649.3508	0.0016	
0.716 (0 1 0 9 1)			
0.254 (0 1 0 9 3)			
1815.0604	1815.0605	-0.0002	
0.274 (0 1 0 9 3)			
0.459 (0 1 0 9 5)			
1936.4308	1936.4317	-0.0009	
0.388 (0 1 0 9 3)			
0.332 (0 1 0 9 7)			
2022.3028	2022.3042	-0.0014	
0.300 (0 1 0 9 5)			
0.539 (0 1 0 9 7)			
2106.1706	2106.1699	0.0007	
0.919 (0 1 0 9 9)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
1649.3518	1649.3508	0.0009	
0.407 (0 1 0 9 0)			
0.486 (0 1 0 9 2)			
1815.0562	1815.0582	-0.0020	
0.552 (0 1 0 9 4)			
1935.6460	1935.6475	-0.0015	
0.479 (0 1 0 9 6)			
2002.3590	2002.3598	-0.0008	
0.302 (0 1 0 9 2)			
0.285 (0 1 0 9 4)			
2063.4478	2063.4492	-0.0013	
0.749 (0 1 0 9 8)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
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	1737.8237	1737.8251	-0.0014
0.606 (0 1 0 9 3)			
	1881.1441	1881.1455	-0.0014
0.300 (0 1 0 9 1)			
0.508 (0 1 0 9 5)			
	1976.0990	1976.0996	-0.0006
0.414 (0 1 0 9 1)			
0.340 (0 1 0 9 7)			
	2027.6844	2027.6843	0.0002
0.293 (0 1 0 9 5)			
0.407 (0 1 0 9 7)			
	2106.1932	2106.1923	0.0009
0.918 (0 1 0 9 9)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	1747.7061	1747.7049	0.0012
0.387 (0 1 0 10 0)			
0.485 (0 1 0 10 2)			
	1933.9589	1933.9580	0.0009
0.494 (0 1 0 10 4)			
0.273 (0 1 0 10 6)			
	2075.1658	2075.1657	0.0001
0.415 (0 1 0 10 6)			
	2164.7661	2164.7678	-0.0018
0.335 (0 1 0 10 2)			
0.271 (0 1 0 10 8)			
	2221.9548	2221.9557	-0.0009
0.290 (0 1 0 10 6)			
0.450 (0 1 0 10 8)			
	2310.1192	2310.1183	0.0009
0.916 (0 1 0 10 10)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	1846.5259	1846.5259	0.0000
0.583 (0 1 0 10 3)			
	2010.1937	2010.1919	0.0018
0.256 (0 1 0 10 1)			
0.424 (0 1 0 10 5)			
0.255 (0 1 0 10 7)			
	2127.7584	2127.7569	0.0015
0.367 (0 1 0 10 1)			
0.404 (0 1 0 10 7)			
	2190.9163	2190.9146	0.0017
0.274 (0 1 0 10 5)			
	2263.6987	2263.6984	0.0003
0.759 (0 1 0 10 9)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	1846.5241	1846.5260	-0.0019

0.473 (0 1 0 10 2)			
0.442 (0 1 0 10 4)			
	2010.2033	2010.2045	-0.0012
0.360 (0 1 0 10 2)			
0.471 (0 1 0 10 6)			
	2129.8824	2129.8823	0.0002
0.376 (0 1 0 10 4)			
0.321 (0 1 0 10 8)			
	2218.9263	2218.9258	0.0005
0.297 (0 1 0 10 6)			
0.525 (0 1 0 10 8)			
	2310.1094	2310.1084	0.0010
0.916 (0 1 0 10 10)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	1747.7055	1747.7049	0.0005
0.689 (0 1 0 10 1)			
0.269 (0 1 0 10 3)			
	1933.9553	1933.9585	-0.0032
0.486 (0 1 0 10 5)			
	2075.3732	2075.3739	-0.0007
0.379 (0 1 0 10 3)			
0.421 (0 1 0 10 7)			
	2176.0090	2176.0093	-0.0003
0.358 (0 1 0 10 5)			
0.293 (0 1 0 10 7)			
	2263.4313	2263.4322	-0.0010
0.769 (0 1 0 10 9)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	1964.4660	1964.4658	0.0003
0.429 (0 1 0 11 2)			
0.457 (0 1 0 11 4)			
	0.0000	2148.3405	0.0000
0.353 (0 1 0 11 2)			
0.475 (0 1 0 11 6)			
	2287.5987	2287.5955	0.0031
0.340 (0 1 0 11 4)			
0.401 (0 1 0 11 8)			
	2388.9569	2388.9554	0.0015
0.347 (0 1 0 11 6)			
0.273 (0 1 0 11 8)			
	2483.5093	2483.5078	0.0016
0.765 (0 1 0 11 10)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	1855.3157	1855.3150	0.0007
0.666 (0 1 0 11 1)			
0.282 (0 1 0 11 3)			

	2062.0534	2062.0523	0.0011
0.491 (0 1 0 11 5)	2223.4783	2223.4774	0.0009
0.351 (0 1 0 11 3)			
0.449 (0 1 0 11 7)	2341.6063	2341.6084	-0.0021
0.349 (0 1 0 11 5)			
0.307 (0 1 0 11 9)	2435.1272	2435.1286	-0.0014
0.294 (0 1 0 11 7)			
0.517 (0 1 0 11 9)	2533.0499	2533.0502	-0.0003
0.913 (0 1 0 11 11)			

SYMMETRY B1

EIGENSTATE	E _{exp}	E _{calc}	Residual
	1855.3150	1855.3150	0.0001
0.370 (0 1 0 11 0)			
0.483 (0 1 0 11 2)	2062.0492	2062.0522	-0.0030
0.434 (0 1 0 11 4)			
0.323 (0 1 0 11 6)	2223.4245	2223.4240	0.0004
0.309 (0 1 0 11 6)			
0.277 (0 1 0 11 8)	2336.7004	2336.6984	0.0021
0.292 (0 1 0 11 2)			
0.333 (0 1 0 11 8)	2398.8974	2398.8955	0.0018
0.280 (0 1 0 11 6)	2483.6316	2483.6311	0.0005
0.761 (0 1 0 11 10)			

SYMMETRY B2

EIGENSTATE	E _{exp}	E _{calc}	Residual
	1964.4630	1964.4658	-0.0028
0.558 (0 1 0 11 3)			
0.261 (0 1 0 11 5)	2148.3371	2148.3376	-0.0005
0.334 (0 1 0 11 5)			
0.324 (0 1 0 11 7)	2286.9438	2286.9422	0.0016
0.308 (0 1 0 11 1)			
0.337 (0 1 0 11 7)	2370.4654	2370.4622	0.0032
0.302 (0 1 0 11 1)			
0.278 (0 1 0 11 3)	2436.7141	2436.7127	0.0014
0.290 (0 1 0 11 7)			
0.478 (0 1 0 11 9)	2533.0542	2533.0547	-0.0005
0.913 (0 1 0 11 11)			

SYMMETRY A1				
EIGENSTATE	Eexp	Ecalc	Residual	
1972.1659	1972.1655	0.0004		
0.356 (0 1 0 12 0)				
0.479 (0 1 0 12 2)				
2199.3274	2199.3275	-0.0001		
0.378 (0 1 0 12 4)				
0.360 (0 1 0 12 6)				
2380.6154	2380.6135	0.0019		
0.348 (0 1 0 12 8)				
2515.8462	2515.8475	-0.0013		
0.275 (0 1 0 12 8)				
0.0000	2593.7321	0.0000		
2671.5311	2671.5305	0.0006		
0.291 (0 1 0 12 8)				
0.492 (0 1 0 12 10)				
2774.5806	2774.5824	-0.0018		
0.908 (0 1 0 12 12)				

SYMMETRY A2				
EIGENSTATE	Eexp	Ecalc	Residual	
2091.6297	2091.6297	0.0000		
0.532 (0 1 0 12 3)				
0.288 (0 1 0 12 5)				
0.0000	2295.5896	0.0000		
0.253 (0 1 0 12 5)				
0.373 (0 1 0 12 7)				
2454.3542	2454.3506	0.0036		
0.263 (0 1 0 12 1)				
0.284 (0 1 0 12 9)				
2561.8058	2561.8021	0.0037		
0.340 (0 1 0 12 1)				
0.273 (0 1 0 12 9)				
2626.9275	2626.9237	0.0038		
0.294 (0 1 0 12 7)				
0.0000	2722.8182	0.0000		
0.758 (0 1 0 12 11)				

SYMMETRY B1				
EIGENSTATE	Eexp	Ecalc	Residual	
2091.6266	2091.6297	-0.0031		
0.392 (0 1 0 12 2)				
0.464 (0 1 0 12 4)				
2295.5903	2295.5903	0.0000		
0.342 (0 1 0 12 2)				
0.450 (0 1 0 12 6)				
2454.5403	2454.5390	0.0014		
0.282 (0 1 0 12 4)				
0.412 (0 1 0 12 8)				
2571.5745	2571.5749	-0.0004		
0.325 (0 1 0 12 6)				

0.295 (0 1 0 12 10)	2670.7437	2670.7429	0.0008
0.293 (0 1 0 12 8)			
0.511 (0 1 0 12 10)	2774.5781	2774.5803	-0.0022
0.908 (0 1 0 12 12)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
1972.1653	1972.1655	-0.0003	
0.645 (0 1 0 12 1)			
0.292 (0 1 0 12 3)	2199.3248	2199.3275	-0.0027
0.482 (0 1 0 12 5)	2380.6285	2380.6271	0.0013
0.315 (0 1 0 12 3)			
0.426 (0 1 0 12 7)	2517.6120	2517.6122	-0.0002
0.291 (0 1 0 12 5)			
0.376 (0 1 0 12 9)	2620.9212	2620.9212	0.0000
0.338 (0 1 0 12 7)			
0.261 (0 1 0 12 9)	0.0000	2722.7615	0.0000
0.760 (0 1 0 12 11)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2228.0009	2228.0015	-0.0006	
0.360 (0 1 0 13 2)			
0.466 (0 1 0 13 4)	0.0000	2451.9384	0.0000
0.329 (0 1 0 13 2)			
0.410 (0 1 0 13 6)	2630.4622	2630.4609	0.0013
0.368 (0 1 0 13 8)	0.0000	2765.2455	0.0000
0.258 (0 1 0 13 4)			
0.252 (0 1 0 13 6)			
0.352 (0 1 0 13 10)	0.0000	2871.8862	0.0000
0.332 (0 1 0 13 8)			
0.253 (0 1 0 13 10)	0.0000	2980.8093	0.0000
0.753 (0 1 0 13 12)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2098.2400	2098.2398	0.0002	
0.626 (0 1 0 13 1)			
0.299 (0 1 0 13 3)	2345.7683	2345.7680	0.0003

0.463 (0 1 0 13 5)	2546.7899	2546.7871	0.0028
0.278 (0 1 0 13 3)			
0.374 (0 1 0 13 7)	2703.0520	2703.0584	-0.0064
0.258 (0 1 0 13 3)			
0.373 (0 1 0 13 9)	0.0000	2819.8116	0.0000
0.306 (0 1 0 13 7)			
0.288 (0 1 0 13 11)	0.0000	2925.5089	0.0000
0.293 (0 1 0 13 9)			
0.503 (0 1 0 13 11)	0.0000	3034.2698	0.0000
0.902 (0 1 0 13 13)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	2098.2394	2098.2398	-0.0004
0.343 (0 1 0 13 0)			
0.475 (0 1 0 13 2)	2345.7669	2345.7680	-0.0011
0.327 (0 1 0 13 4)			
0.385 (0 1 0 13 6)	2546.7855	2546.7835	0.0020
0.387 (0 1 0 13 8)	2702.4801	2702.4848	-0.0048
0.277 (0 1 0 13 10)	0.0000	2802.8625	0.0000
0.283 (0 1 0 13 2)	2875.2113	2875.2093	0.0020
0.307 (0 1 0 13 8)	0.0000	2980.8355	0.0000
0.752 (0 1 0 13 12)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	2227.9978	2228.0015	-0.0037
0.507 (0 1 0 13 3)			
0.310 (0 1 0 13 5)	2451.9399	2451.9382	0.0016
0.400 (0 1 0 13 7)	2630.4066	2630.4076	-0.0010
0.251 (0 1 0 13 5)			
0.350 (0 1 0 13 9)	0.0000	2761.0835	0.0000
0.318 (0 1 0 13 1)	2835.3900	2835.3926	-0.0026
	0.0000	2925.8885	0.0000
0.292 (0 1 0 13 9)			
0.494 (0 1 0 13 11)	3034.2733	3034.2708	0.0025

0.902 (0 1 0 13 13)

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2233.5200	2233.5197	0.0003	
0.332 (0 1 0 14 0)			
0.470 (0 1 0 14 2)			
2501.3569	2501.3558	0.0011	
0.282 (0 1 0 14 4)			
0.400 (0 1 0 14 6)			
0.0000	2721.9376	0.0000	
0.251 (0 1 0 14 4)			
0.398 (0 1 0 14 8)			
0.0000	2897.3005	0.0000	
0.263 (0 1 0 14 6)			
0.340 (0 1 0 14 10)			
0.0000	3021.8133	0.0000	
0.272 (0 1 0 14 2)			
0.0000	3096.3105	0.0000	
0.0000	3199.2737	0.0000	
0.294 (0 1 0 14 10)			
0.488 (0 1 0 14 12)			
0.0000	3311.6773	0.0000	
0.895 (0 1 0 14 14)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2373.5629	2373.5634	-0.0005	
0.483 (0 1 0 14 3)			
0.327 (0 1 0 14 5)			
2617.3732	2617.3674	0.0058	
0.410 (0 1 0 14 7)			
2815.2619	2815.2637	-0.0018	
0.272 (0 1 0 14 5)			
0.377 (0 1 0 14 9)			
0.0000	2967.2053	0.0000	
0.276 (0 1 0 14 1)			
0.260 (0 1 0 14 11)			
0.0000	3060.2943	0.0000	
0.0000	3143.4644	0.0000	
0.315 (0 1 0 14 9)			
0.0000	3257.2550	0.0000	
0.744 (0 1 0 14 13)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2373.5597	2373.5634	-0.0037	
0.333 (0 1 0 14 2)			
0.464 (0 1 0 14 4)			
2617.3705	2617.3675	0.0031	
0.316 (0 1 0 14 2)			
0.363 (0 1 0 14 6)			

0.279 (0 1 0 14 8)	0.0000	2815.2788	0.0000
0.296 (0 1 0 14 8)	0.0000	2968.7430	0.0000
0.270 (0 1 0 14 4)			
0.338 (0 1 0 14 10)	0.0000	3086.3714	0.0000
0.294 (0 1 0 14 8)			
0.286 (0 1 0 14 12)	0.0000	3199.0941	0.0000
0.295 (0 1 0 14 10)			
0.492 (0 1 0 14 12)	0.0000	3311.6769	0.0000
0.895 (0 1 0 14 14)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2233.5193	2233.5197	-0.0004	
0.609 (0 1 0 14 1)			
0.305 (0 1 0 14 3)	2501.3553	2501.3559	-0.0005
0.440 (0 1 0 14 5)	2721.9408	2721.9386	0.0022
0.309 (0 1 0 14 7)			
0.274 (0 1 0 14 9)	2897.4642	2897.4793	-0.0152
0.263 (0 1 0 14 3)			
0.314 (0 1 0 14 9)	0.0000	3030.4123	0.0000
0.259 (0 1 0 14 5)			
0.333 (0 1 0 14 11)	0.0000	3141.7394	0.0000
0.328 (0 1 0 14 9)	0.0000	3257.2429	0.0000
0.744 (0 1 0 14 13)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2528.2960	2528.2965	-0.0005	
0.309 (0 1 0 15 2)			
0.460 (0 1 0 15 4)	0.0000	2791.8578	0.0000
0.303 (0 1 0 15 2)			
0.314 (0 1 0 15 6)			
0.312 (0 1 0 15 8)	0.0000	3008.9625	0.0000
0.295 (0 1 0 15 10)	0.0000	3181.3309	0.0000
0.260 (0 1 0 15 4)			
0.268 (0 1 0 15 10)	0.0000	3313.1181	0.0000
0.253 (0 1 0 15 6)			

0.319 (0 1 0 15 12)	0.0000	3430.2678	0.0000
0.326 (0 1 0 15 10)	0.0000	3551.6328	0.0000
0.733 (0 1 0 15 14)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2377.9860	2377.9858	0.0003	
0.594 (0 1 0 15 1)			
0.310 (0 1 0 15 3)			
2666.0734	2666.0714	0.0021	
0.413 (0 1 0 15 5)			
0.276 (0 1 0 15 7)			
2906.0662	2906.0636	0.0026	
0.316 (0 1 0 15 9)			
0.0000	3100.6944	0.0000	
0.257 (0 1 0 15 3)			
0.252 (0 1 0 15 11)			
0.0000	3251.3727	0.0000	
0.261 (0 1 0 15 5)			
0.308 (0 1 0 15 11)			
0.0000	3371.2757	0.0000	
0.286 (0 1 0 15 9)			
0.288 (0 1 0 15 13)			
0.0000	3491.1078	0.0000	
0.298 (0 1 0 15 11)			
0.479 (0 1 0 15 13)			
0.0000	3606.3478	0.0000	
0.886 (0 1 0 15 15)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2377.9854	2377.9858	-0.0004	
0.322 (0 1 0 15 0)			
0.466 (0 1 0 15 2)			
2666.0718	2666.0714	0.0005	
0.406 (0 1 0 15 6)			
2906.0653	2906.0633	0.0020	
0.262 (0 1 0 15 4)			
0.385 (0 1 0 15 8)			
0.0000	3100.6392	0.0000	
0.265 (0 1 0 15 6)			
0.355 (0 1 0 15 10)			
0.0000	3247.7098	0.0000	
0.0000	3334.9724	0.0000	
0.0000	3431.1255	0.0000	
0.319 (0 1 0 15 10)			
0.0000	3551.6385	0.0000	
0.733 (0 1 0 15 14)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2528.2929	2528.2965	-0.0036	
0.461 (0 1 0 15 3)			
0.341 (0 1 0 15 5)			
2791.8621	2791.8578	0.0043	
0.405 (0 1 0 15 7)			
0.0000	3008.9582	0.0000	
0.274 (0 1 0 15 5)			
0.369 (0 1 0 15 9)			
0.0000	3180.8006	0.0000	
0.251 (0 1 0 15 7)			
0.321 (0 1 0 15 11)			
0.0000	3297.5374	0.0000	
0.286 (0 1 0 15 1)			
0.0000	3377.0491	0.0000	
0.251 (0 1 0 15 13)			
0.0000	3491.1921	0.0000	
0.297 (0 1 0 15 11)			
0.477 (0 1 0 15 13)			
0.0000	3606.3480	0.0000	
0.886 (0 1 0 15 15)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2531.6175	2531.6173	0.0002	
0.313 (0 1 0 16 0)			
0.461 (0 1 0 16 2)			
2839.8962	2839.8934	0.0028	
0.407 (0 1 0 16 6)			
0.0000	3099.1409	0.0000	
0.265 (0 1 0 16 4)			
0.358 (0 1 0 16 8)			
0.0000	3312.6235	0.0000	
0.331 (0 1 0 16 10)			
0.0000	3480.2947	0.0000	
0.296 (0 1 0 16 12)			
0.0000	3588.4549	0.0000	
0.0000	3677.5787	0.0000	
0.255 (0 1 0 16 10)			
0.272 (0 1 0 16 14)			
0.0000	3801.1637	0.0000	
0.300 (0 1 0 16 12)			
0.461 (0 1 0 16 14)			
0.0000	3917.7958	0.0000	
0.876 (0 1 0 16 16)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2692.1803	2692.1805	-0.0002	
0.440 (0 1 0 16 3)			
0.351 (0 1 0 16 5)			
0.0000	2975.3874	0.0000	

0.391 (0 1 0 16 7)	0.0000	3211.4907	0.0000
0.262 (0 1 0 16 5)			
0.337 (0 1 0 16 9)	0.0000	3402.4842	0.0000
0.327 (0 1 0 16 11)	0.0000	3543.0748	0.0000
0.285 (0 1 0 16 1)	0.0000	3627.9643	0.0000
	0.0000	3737.5729	0.0000
0.321 (0 1 0 16 11)	0.0000	3863.5375	0.0000
0.720 (0 1 0 16 15)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2692.1771	2692.1805	-0.0034	
0.289 (0 1 0 16 2)			
0.454 (0 1 0 16 4)	0.0000	2975.3874	0.0000
0.290 (0 1 0 16 2)			
0.268 (0 1 0 16 6)			
0.336 (0 1 0 16 8)	0.0000	3211.4921	0.0000
0.330 (0 1 0 16 10)	0.0000	3402.6625	0.0000
0.254 (0 1 0 16 12)	0.0000	3550.8283	0.0000
0.285 (0 1 0 16 12)	0.0000	3674.4694	0.0000
0.281 (0 1 0 16 10)			
0.293 (0 1 0 16 14)	0.0000	3801.1243	0.0000
0.301 (0 1 0 16 12)			
0.462 (0 1 0 16 14)	0.0000	3917.7957	0.0000
0.876 (0 1 0 16 16)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2531.6168	2531.6173	-0.0004	
0.580 (0 1 0 16 1)			
0.314 (0 1 0 16 3)	2839.8946	2839.8934	0.0012
0.386 (0 1 0 16 5)			
0.298 (0 1 0 16 7)	3099.1418	3099.1410	0.0008
0.342 (0 1 0 16 9)	0.0000	3312.6405	0.0000
0.302 (0 1 0 16 11)	0.0000	3481.6997	0.0000
	0.0000	3613.4193	0.0000

0.312 (0 1 0 16 13)	0.0000	3737.1578	0.0000
0.324 (0 1 0 16 11)	0.0000	3863.5348	0.0000
0.720 (0 1 0 16 15)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2865.1938	2865.1938	0.0000	
0.271 (0 1 0 17 2)			
0.447 (0 1 0 17 4)	0.0000	3167.9321	0.0000
0.277 (0 1 0 17 2)			
0.350 (0 1 0 17 8)	0.0000	3422.8462	0.0000
0.344 (0 1 0 17 10)	0.0000	3632.6023	0.0000
0.300 (0 1 0 17 12)	0.0000	3798.3442	0.0000
	0.0000	3931.3765	0.0000
0.309 (0 1 0 17 14)	0.0000	4062.0317	0.0000
0.322 (0 1 0 17 12)	0.0000	4192.4459	0.0000
0.705 (0 1 0 17 16)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2694.3922	2694.3921	0.0001	
0.567 (0 1 0 17 1)			
0.316 (0 1 0 17 3)	3022.8022	3022.7993	0.0029
0.359 (0 1 0 17 5)			
0.315 (0 1 0 17 7)	0.0000	3301.1468	0.0000
0.353 (0 1 0 17 9)	0.0000	3533.2900	0.0000
0.327 (0 1 0 17 11)	0.0000	3720.8223	0.0000
0.251 (0 1 0 17 13)	0.0000	3867.0892	0.0000
0.269 (0 1 0 17 13)	0.0000	3995.7813	0.0000
0.277 (0 1 0 17 11)			
0.301 (0 1 0 17 15)	0.0000	4128.6787	0.0000
0.304 (0 1 0 17 13)			
0.442 (0 1 0 17 15)	0.0000	4245.5180	0.0000
0.864 (0 1 0 17 17)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2694.3916	2694.3921	-0.0005	
0.305 (0 1 0 17 0)			
0.456 (0 1 0 17 2)			
3022.8006	3022.7993	0.0013	
0.403 (0 1 0 17 6)			
3301.1451	3301.1469	-0.0018	
0.263 (0 1 0 17 4)			
0.321 (0 1 0 17 8)			
0.0000	3533.2852	0.0000	
0.281 (0 1 0 17 10)			
0.0000	3720.3112	0.0000	
0.298 (0 1 0 17 12)			
0.0000	3852.5835	0.0000	
0.251 (0 1 0 17 2)			
0.0000	3940.1668	0.0000	
0.251 (0 1 0 17 14)			
0.0000	4062.2294	0.0000	
0.320 (0 1 0 17 12)			
0.0000	4192.4473	0.0000	
0.705 (0 1 0 17 16)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2865.1906	2865.1938	-0.0032	
0.421 (0 1 0 17 3)			
0.358 (0 1 0 17 5)			
0.0000	3167.9321	0.0000	
0.370 (0 1 0 17 7)			
0.0000	3422.8456	0.0000	
0.289 (0 1 0 17 9)			
0.0000	3632.5415	0.0000	
0.290 (0 1 0 17 11)			
0.0000	3794.9853	0.0000	
0.257 (0 1 0 17 1)			
0.266 (0 1 0 17 13)			
0.0000	3895.4331	0.0000	
0.0000	3997.3694	0.0000	
0.264 (0 1 0 17 11)			
0.290 (0 1 0 17 15)			
0.0000	4128.6972	0.0000	
0.304 (0 1 0 17 13)			
0.442 (0 1 0 17 15)			
0.0000	4245.5180	0.0000	
0.864 (0 1 0 17 17)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2866.2867	2866.2867	0.0000	
0.298 (0 1 0 18 0)			
0.451 (0 1 0 18 2)			
0.0000	3214.7649	0.0000	

0.396 (0 1 0 18 6)	0.0000	3512.0541	0.0000
0.256 (0 1 0 18 4)			
0.281 (0 1 0 18 8)			
0.274 (0 1 0 18 10)	0.0000	3762.6207	0.0000
0.257 (0 1 0 18 12)	0.0000	3968.2960	0.0000
0.253 (0 1 0 18 12)	0.0000	4123.9232	0.0000
	0.0000	4219.7158	0.0000
	0.0000	4335.7236	0.0000
0.266 (0 1 0 18 12)			
0.305 (0 1 0 18 16)	0.0000	4473.2374	0.0000
0.307 (0 1 0 18 14)			
0.419 (0 1 0 18 16)	0.0000	4588.9533	0.0000
0.849 (0 1 0 18 18)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
3047.3138	3047.3136	0.0002	
0.403 (0 1 0 18 3)			
0.364 (0 1 0 18 5)	0.0000	3369.4659	0.0000
0.345 (0 1 0 18 7)			
0.254 (0 1 0 18 9)	0.0000	3642.9991	0.0000
0.274 (0 1 0 18 11)	0.0000	3871.0761	0.0000
	0.0000	4053.5105	0.0000
0.268 (0 1 0 18 13)	0.0000	4176.1917	0.0000
	0.0000	4271.8619	0.0000
0.276 (0 1 0 18 15)	0.0000	4404.5300	0.0000
0.318 (0 1 0 18 13)	0.0000	4537.8612	0.0000
0.687 (0 1 0 18 17)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
3047.3107	3047.3136	-0.0030	
0.255 (0 1 0 18 2)			
0.439 (0 1 0 18 4)	0.0000	3369.4659	0.0000
0.266 (0 1 0 18 2)			
0.357 (0 1 0 18 8)	0.0000	3642.9997	0.0000
0.339 (0 1 0 18 10)	0.0000	3871.0991	0.0000

0.314 (0 1 0 18 12)	0.0000	4054.8591	0.0000
	0.0000	4200.2286	0.0000
0.258 (0 1 0 18 14)	0.0000	4334.9404	0.0000
0.272 (0 1 0 18 12)			
0.310 (0 1 0 18 16)	0.0000	4473.2287	0.0000
0.307 (0 1 0 18 14)			
0.419 (0 1 0 18 16)	0.0000	4588.9533	0.0000
0.849 (0 1 0 18 18)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2866.2860	2866.2867	-0.0007	
0.556 (0 1 0 18 1)			
0.319 (0 1 0 18 3)	0.0000	3214.7649	0.0000
0.333 (0 1 0 18 5)			
0.328 (0 1 0 18 7)	0.0000	3512.0540	0.0000
0.353 (0 1 0 18 9)	0.0000	3762.6210	0.0000
0.327 (0 1 0 18 11)	0.0000	3968.4753	0.0000
0.290 (0 1 0 18 13)	0.0000	4131.1130	0.0000
	0.0000	4266.9743	0.0000
0.310 (0 1 0 18 15)	0.0000	4404.4366	0.0000
0.319 (0 1 0 18 13)	0.0000	4537.8606	0.0000
0.687 (0 1 0 18 17)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
3238.5157	3238.5156	0.0001	
0.430 (0 1 0 19 4)			
0.252 (0 1 0 19 6)	0.0000	3579.9609	0.0000
0.255 (0 1 0 19 2)			
0.357 (0 1 0 19 8)	0.0000	3871.9236	0.0000
0.321 (0 1 0 19 10)	0.0000	4118.1270	0.0000
0.301 (0 1 0 19 12)	0.0000	4319.9221	0.0000
0.278 (0 1 0 19 14)	0.0000	4479.9957	0.0000
	0.0000	4620.0937	0.0000
0.313 (0 1 0 19 16)			

	0.0000	4763.8345	0.0000
0.315 (0 1 0 19 14)			
0.262 (0 1 0 19 18)			
	0.0000	4899.1771	0.0000
0.250 (0 1 0 19 16)			
0.668 (0 1 0 19 18)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	3047.2762	3047.2758	0.0004
0.545 (0 1 0 19 1)			
0.320 (0 1 0 19 3)			
	0.0000	3415.7646	0.0000
0.308 (0 1 0 19 5)			
0.337 (0 1 0 19 7)			
	0.0000	3731.8327	0.0000
0.343 (0 1 0 19 9)			
	0.0000	4000.6088	0.0000
0.307 (0 1 0 19 11)			
	0.0000	4224.5530	0.0000
0.296 (0 1 0 19 13)			
	0.0000	4404.5076	0.0000
	0.0000	4550.3210	0.0000
0.253 (0 1 0 19 15)			
	0.0000	4691.5595	0.0000
0.266 (0 1 0 19 13)			
0.320 (0 1 0 19 17)			
	0.0000	4834.2371	0.0000
0.309 (0 1 0 19 15)			
0.393 (0 1 0 19 17)			
	0.0000	4947.4751	0.0000
0.832 (0 1 0 19 19)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	3047.2755	3047.2758	-0.0003
0.291 (0 1 0 19 0)			
0.446 (0 1 0 19 2)			
	0.0000	3415.7647	0.0000
0.386 (0 1 0 19 6)			
	0.0000	3731.8330	0.0000
0.296 (0 1 0 19 10)			
	0.0000	4000.6109	0.0000
0.288 (0 1 0 19 12)			
	0.0000	4224.4946	0.0000
	0.0000	4401.3213	0.0000
	0.0000	4514.7182	0.0000
	0.0000	4622.6485	0.0000
0.295 (0 1 0 19 16)			
	0.0000	4763.8785	0.0000
0.315 (0 1 0 19 14)			
0.261 (0 1 0 19 18)			

	0.0000	4899.1775	0.0000
0.250 (0 1 0 19 16)			
0.668 (0 1 0 19 18)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	3238.5125	3238.5156	-0.0031
0.387 (0 1 0 19 3)			
0.367 (0 1 0 19 5)			
	0.0000	3579.9609	0.0000
0.318 (0 1 0 19 7)			
0.275 (0 1 0 19 9)			
	0.0000	3871.9224	0.0000
0.298 (0 1 0 19 11)			
	0.0000	4118.1149	0.0000
0.265 (0 1 0 19 13)			
	0.0000	4319.3966	0.0000
	0.0000	4466.2343	0.0000
0.257 (0 1 0 19 1)			
	0.0000	4562.4823	0.0000
	0.0000	4691.9374	0.0000
0.263 (0 1 0 19 13)			
0.318 (0 1 0 19 17)			
	0.0000	4834.2413	0.0000
0.309 (0 1 0 19 15)			
0.393 (0 1 0 19 17)			
	0.0000	4947.4751	0.0000
0.832 (0 1 0 19 19)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	3237.3346	3237.3319	0.0027
0.285 (0 1 0 20 0)			
0.442 (0 1 0 20 2)			
	0.0000	3625.7712	0.0000
0.375 (0 1 0 20 6)			
	0.0000	3960.4513	0.0000
0.311 (0 1 0 20 10)			
	0.0000	4247.2282	0.0000
0.303 (0 1 0 20 12)			
	0.0000	4488.9996	0.0000
0.266 (0 1 0 20 14)			
	0.0000	4685.2833	0.0000
	0.0000	4821.6801	0.0000
	0.0000	4924.3341	0.0000
	0.0000	5065.3270	0.0000
0.257 (0 1 0 20 14)			
0.330 (0 1 0 20 18)			
	0.0000	5211.0262	0.0000
0.309 (0 1 0 20 16)			
0.364 (0 1 0 20 18)			
	0.0000	5320.3734	0.0000

0.811 (0 1 0 20 20)

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	3438.7736	0.0000	
0.372 (0 1 0 20 3)			
0.369 (0 1 0 20 5)			
0.0000	3799.3870	0.0000	
0.291 (0 1 0 20 7)			
0.291 (0 1 0 20 9)			
0.0000	4109.5830	0.0000	
0.311 (0 1 0 20 11)			
0.0000	4373.6519	0.0000	
0.289 (0 1 0 20 13)			
0.0000	4593.1200	0.0000	
0.0000	4762.7664	0.0000	
0.0000	4869.5246	0.0000	
0.0000	4991.7674	0.0000	
0.308 (0 1 0 20 17)			
0.0000	5139.7093	0.0000	
0.309 (0 1 0 20 15)			
0.278 (0 1 0 20 19)			
0.0000	5275.7191	0.0000	
0.261 (0 1 0 20 17)			
0.647 (0 1 0 20 19)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	3438.7736	0.0000	
0.421 (0 1 0 20 4)			
0.262 (0 1 0 20 6)			
0.0000	3799.3872	0.0000	
0.353 (0 1 0 20 8)			
0.0000	4109.5850	0.0000	
0.294 (0 1 0 20 10)			
0.0000	4373.6625	0.0000	
0.267 (0 1 0 20 12)			
0.0000	4593.3249	0.0000	
0.275 (0 1 0 20 14)			
0.0000	4769.6367	0.0000	
0.0000	4917.3867	0.0000	
0.251 (0 1 0 20 16)			
0.0000	5065.1468	0.0000	
0.259 (0 1 0 20 14)			
0.331 (0 1 0 20 18)			
0.0000	5211.0242	0.0000	
0.309 (0 1 0 20 16)			
0.364 (0 1 0 20 18)			
0.0000	5320.3734	0.0000	
0.811 (0 1 0 20 20)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
3237.3340	3237.3319	0.0020	
0.535 (0 1 0 20 1)			
0.321 (0 1 0 20 3)			
0.0000	3625.7711	0.0000	
0.285 (0 1 0 20 5)			
0.343 (0 1 0 20 7)			
0.0000	3960.4507	0.0000	
0.326 (0 1 0 20 9)			
0.0000	4247.2237	0.0000	
0.273 (0 1 0 20 11)			
0.0000	4489.0135	0.0000	
0.272 (0 1 0 20 13)			
0.0000	4686.6131	0.0000	
0.264 (0 1 0 20 15)			
0.0000	4845.0514	0.0000	
0.0000	4990.4862	0.0000	
0.318 (0 1 0 20 17)			
0.0000	5139.6884	0.0000	
0.309 (0 1 0 20 15)			
0.278 (0 1 0 20 19)			
0.0000	5275.7190	0.0000	
0.261 (0 1 0 20 17)			
0.647 (0 1 0 20 19)			

POLYAD P = 2

SYMMETRY A1			
EIGENSTATE	Eexp	Ecalc	Residual
2647.5334	2647.5378	-0.0044	
1.000 (0 0 1 1 1)			

SYMMETRY A2			
EIGENSTATE	Eexp	Ecalc	Residual
2369.6858	2369.6913	-0.0055	
0.998 (0 2 0 1 1)			
2629.2678	2629.2700	-0.0022	
0.998 (1 0 0 1 1)			
2642.0688	2642.0726	-0.0038	
1.000 (0 0 1 1 0)			

SYMMETRY B1			
EIGENSTATE	Eexp	Ecalc	Residual
2368.0151	2368.0206	-0.0055	
0.998 (0 2 0 1 0)			
2627.9574	2627.9590	-0.0016	
0.998 (1 0 0 1 0)			
2643.2767	2643.2815	-0.0048	
1.000 (0 0 1 1 1)			

SYMMETRY B2

	EIGENSTATE	Eexp	Ecalc	Residual
	2374.5212	2374.5263	-0.0051	
0.998	(0 2 0 1 1)			
	2633.5002	2633.5019	-0.0017	
0.998	(1 0 0 1 1)			

SYMMETRY A1

	EIGENSTATE	Eexp	Ecalc	Residual
	2392.5720	2392.5771	-0.0051	
0.847	(0 2 0 2 0)			
	2415.9544	2415.9576	-0.0032	
0.847	(0 2 0 2 2)			
	2651.8677	2651.8700	-0.0023	
0.840	(1 0 0 2 0)			
	2666.2032	2666.2075	-0.0043	
0.993	(0 0 1 2 1)			
	2671.9588	2671.9600	-0.0012	
0.833	(1 0 0 2 2)			

SYMMETRY A2

	EIGENSTATE	Eexp	Ecalc	Residual
	2407.4391	2407.4422	-0.0031	
0.998	(0 2 0 2 1)			
	2664.8090	2664.8099	-0.0009	
0.997	(1 0 0 2 1)			
	2682.6306	2682.6344	-0.0038	
0.999	(0 0 1 2 2)			

SYMMETRY B1

	EIGENSTATE	Eexp	Ecalc	Residual
	2412.4321	2412.4363	-0.0042	
0.998	(0 2 0 2 2)			
	2668.7250	2668.7267	-0.0017	
0.996	(1 0 0 2 2)			
	2679.0204	2679.0234	-0.0030	
0.999	(0 0 1 2 1)			

SYMMETRY B2

	EIGENSTATE	Eexp	Ecalc	Residual
	2392.9519	2392.9568	-0.0049	
0.998	(0 2 0 2 1)			
	2652.1341	2652.1356	-0.0015	
0.998	(1 0 0 2 1)			
	2666.0090	2666.0129	-0.0039	
0.836	(0 0 1 2 0)			
	2685.8946	2685.8987	-0.0041	
0.835	(0 0 1 2 2)			

SYMMETRY A1

	EIGENSTATE	Eexp	Ecalc	Residual
	2454.5763	2454.5785	-0.0022	
0.998	(0 2 0 3 2)			

	2709.3495	2709.3503	-0.0008
0.997 (1 0 0 3 2)	2722.3319	2722.3347	-0.0028
0.822 (0 0 1 3 1)	2743.8897	2743.8930	-0.0033
0.821 (0 0 1 3 3)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2426.0400	2426.0443	-0.0043	
0.963 (0 2 0 3 1)	2476.6295	2476.6320	-0.0025
0.963 (0 2 0 3 3)	2684.8140	2684.8150	-0.0010
0.961 (1 0 0 3 1)	2698.9839	2698.9875	-0.0036
0.688 (0 0 1 3 0)			
0.312 (0 0 1 3 2)	2727.9202	2727.9214	-0.0012
0.946 (1 0 0 3 3)	2734.6249	2734.6258	-0.0009
0.305 (0 0 1 3 0)			
0.680 (0 0 1 3 2)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2425.9800	2425.9843	-0.0043	
0.700 (0 2 0 3 0)			
0.298 (0 2 0 3 2)	2466.7566	2466.7574	-0.0008
0.298 (0 2 0 3 0)			
0.700 (0 2 0 3 2)	2684.7775	2684.7787	-0.0012
0.692 (1 0 0 3 0)			
0.306 (1 0 0 3 2)	2699.0078	2699.0114	-0.0036
0.961 (0 0 1 3 1)	2720.2225	2720.2232	-0.0007
0.305 (1 0 0 3 0)			
0.690 (1 0 0 3 2)	2741.7223	2741.7266	-0.0043
0.959 (0 0 1 3 3)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2452.7923	2452.7946	-0.0023	
0.846 (0 2 0 3 1)	2478.7931	2478.7946	-0.0015
0.846 (0 2 0 3 3)	2708.0890	2708.0896	-0.0006
0.832 (1 0 0 3 1)	2723.2900	2723.2939	-0.0039

0.975 (0 0 1 3 2)	2730.2247	2730.2246	0.0001
0.810 (1 0 0 3 3)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2468.4508	2468.4546	-0.0038	
0.606 (0 2 0 4 0)			
0.385 (0 2 0 4 2)			
2532.0963	2532.0964	-0.0001	
0.371 (0 2 0 4 0)			
0.514 (0 2 0 4 2)			
2563.4426	2563.4434	-0.0008	
0.877 (0 2 0 4 4)			
2726.8903	2726.8906	-0.0003	
0.599 (1 0 0 4 0)			
0.390 (1 0 0 4 2)			
2741.2159	2741.2185	-0.0026	
0.909 (0 0 1 4 1)			
2782.2891	2782.2893	-0.0002	
0.373 (1 0 0 4 0)			
0.497 (1 0 0 4 2)			
2799.4884	2799.4915	-0.0031	
0.871 (0 0 1 4 3)			
2808.6244	2808.6239	0.0005	
0.824 (1 0 0 4 4)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2507.1380	2507.1394	-0.0014	
0.610 (0 2 0 4 1)			
0.388 (0 2 0 4 3)			
2546.2619	2546.2605	0.0014	
0.387 (0 2 0 4 1)			
0.610 (0 2 0 4 3)			
2760.3761	2760.3765	-0.0004	
0.593 (1 0 0 4 1)			
0.405 (1 0 0 4 3)			
2774.7846	2774.7874	-0.0028	
0.932 (0 0 1 4 2)			
2794.4317	2794.4316	0.0001	
0.404 (1 0 0 4 1)			
0.586 (1 0 0 4 3)			
2820.5793	2820.5832	-0.0039	
0.931 (0 0 1 4 4)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2507.5428	2507.5440	-0.0012	
0.941 (0 2 0 4 2)			
2562.2953	2562.2966	-0.0013	
0.941 (0 2 0 4 4)			

	2760.6231	2760.6232	-0.0001
0.936 (1 0 0 4 2)	2774.6212	2774.6236	-0.0024
0.580 (0 0 1 4 1)			
0.419 (0 0 1 4 3)	2806.3392	2806.3420	-0.0028
0.710 (1 0 0 4 4)	2809.6042	2809.6023	0.0019
0.303 (0 0 1 4 1)			
0.449 (0 0 1 4 3)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2468.4594	2468.4633	-0.0039	
0.913 (0 2 0 4 1)	2536.8762	2536.8762	0.0000
0.913 (0 2 0 4 3)	2726.8937	2726.8950	-0.0013
0.910 (1 0 0 4 1)	2741.2128	2741.2159	-0.0031
0.596 (0 0 1 4 0)			
0.395 (0 0 1 4 2)	2785.7104	2785.7108	-0.0004
0.905 (1 0 0 4 3)	2796.7641	2796.7647	-0.0006
0.371 (0 0 1 4 0)			
0.482 (0 0 1 4 2)	2821.8402	2821.8437	-0.0035
0.847 (0 0 1 4 4)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2570.2037	2570.2039	-0.0002	
0.849 (0 2 0 5 2)	2639.9431	2639.9414	0.0017
0.849 (0 2 0 5 4)	2821.5628	2821.5626	0.0002
0.841 (1 0 0 5 2)	2835.8600	2835.8615	-0.0015
0.425 (0 0 1 5 1)			
0.556 (0 0 1 5 3)	2881.1948	2881.1949	-0.0001
0.819 (1 0 0 5 4)	2889.2580	2889.2563	0.0017
0.528 (0 0 1 5 1)			
0.338 (0 0 1 5 3)	2919.8418	2919.8450	-0.0032
0.871 (0 0 1 5 5)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2520.0971	2520.0998	-0.0027	

0.864 (0 2 0 5 1)	2609.1203	2609.1193	0.0010
0.802 (0 2 0 5 3)	2669.3626	2669.3637	-0.0011
0.931 (0 2 0 5 5)	2778.2880	2778.2876	0.0004
0.860 (1 0 0 5 1)	2792.7647	2792.7670	-0.0023
0.534 (0 0 1 5 0)			
0.441 (0 0 1 5 2)	2855.1471	2855.1467	0.0004
0.791 (1 0 0 5 3)	2868.5848	2868.5857	-0.0009
0.343 (0 0 1 5 0)			
0.412 (0 0 1 5 4)	2901.1623	2901.1643	-0.0020
0.271 (0 0 1 5 2)			
0.459 (0 0 1 5 4)	2907.0488	2907.0459	0.0029
0.766 (1 0 0 5 5)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2520.0961	2520.0986	-0.0025	
0.542 (0 2 0 5 0)			
0.434 (0 2 0 5 2)	2607.6112	2607.6108	0.0004
0.355 (0 2 0 5 0)			
0.281 (0 2 0 5 2)			
0.362 (0 2 0 5 4)	2646.4277	2646.4257	0.0020
0.284 (0 2 0 5 2)			
0.614 (0 2 0 5 4)	2778.2875	2778.2871	0.0004
0.537 (1 0 0 5 0)			
0.438 (1 0 0 5 2)	2792.7650	2792.7672	-0.0022
0.858 (0 0 1 5 1)	2854.2110	2854.2112	-0.0002
0.349 (1 0 0 5 0)			
0.259 (1 0 0 5 2)			
0.388 (1 0 0 5 4)	2869.2186	2869.2203	-0.0017
0.778 (0 0 1 5 3)	2887.8203	2887.8201	0.0002
0.298 (1 0 0 5 2)			
0.570 (1 0 0 5 4)	2919.1767	2919.1801	-0.0034
0.915 (0 0 1 5 5)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
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	2570.1281	2570.1286	-0.0005
0.447 (0 2 0 5 1)			
0.536 (0 2 0 5 3)			
	2630.3955	2630.3941	0.0014
0.533 (0 2 0 5 1)			
0.383 (0 2 0 5 3)			
	2669.9130	2669.9133	-0.0003
0.901 (0 2 0 5 5)			
	2821.5241	2821.5235	0.0006
0.434 (1 0 0 5 1)			
0.547 (1 0 0 5 3)			
	2835.8822	2835.8843	-0.0021
0.836 (0 0 1 5 2)			
	2874.3453	2874.3446	0.0007
0.542 (1 0 0 5 1)			
0.361 (1 0 0 5 3)			
	2894.9210	2894.9236	-0.0026
0.791 (0 0 1 5 4)			
	2907.1970	2907.1957	0.0013
0.840 (1 0 0 5 5)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	2580.9280	2580.9306	-0.0026
0.496 (0 2 0 6 0)			
0.461 (0 2 0 6 2)			
	2691.3386	2691.3377	0.0009
0.309 (0 2 0 6 0)			
0.546 (0 2 0 6 4)			
	2747.9479	2747.9465	0.0014
0.403 (0 2 0 6 2)			
0.340 (0 2 0 6 4)			
	2797.9072	2797.9079	-0.0007
0.914 (0 2 0 6 6)			
	2838.9745	2838.9741	0.0004
0.491 (1 0 0 6 0)			
0.464 (1 0 0 6 2)			
	2853.6421	2853.6432	-0.0011
0.813 (0 0 1 6 1)			
	2934.5503	2934.5493	0.0010
0.302 (1 0 0 6 0)			
0.563 (1 0 0 6 4)			
	2949.0465	2949.0467	-0.0002
0.625 (0 0 1 6 3)			
	2984.4253	2984.4246	0.0007
0.409 (1 0 0 6 2)			
0.308 (1 0 0 6 4)			
	3009.6604	3009.6616	-0.0012
0.739 (0 0 1 6 5)			
	3025.7681	3025.7667	0.0014
0.850 (1 0 0 6 6)			

SYMMETRY A2

EIGENSTATE	E _{exp}	E _{calc}	Residual
2642.1370	2642.1367	0.0003	
0.346 (0 2 0 6 1)			
0.604 (0 2 0 6 3)			
2726.7234	2726.7230	0.0004	
0.543 (0 2 0 6 1)			
0.291 (0 2 0 6 5)			
2767.8134	2767.8112	0.0022	
0.658 (0 2 0 6 5)			
2891.8405	2891.8395	0.0010	
0.336 (1 0 0 6 1)			
0.610 (1 0 0 6 3)			
2906.3286	2906.3291	-0.0005	
0.736 (0 0 1 6 2)			
0.258 (0 0 1 6 4)			
2965.7749	2965.7742	0.0007	
0.535 (1 0 0 6 1)			
0.318 (1 0 0 6 5)			
2982.2474	2982.2481	-0.0007	
0.250 (0 0 1 6 2)			
0.645 (0 0 1 6 4)			
3000.8610	3000.8593	0.0017	
0.590 (1 0 0 6 5)			
3037.4254	3037.4274	-0.0020	
0.904 (0 0 1 6 6)			

SYMMETRY B1

EIGENSTATE	E _{exp}	E _{calc}	Residual
2642.1499	2642.1500	-0.0001	
0.752 (0 2 0 6 2)			
2730.7427	2730.7403	0.0024	
0.690 (0 2 0 6 4)			
2797.6592	2797.6596	-0.0004	
0.926 (0 2 0 6 6)			
2891.8461	2891.8454	0.0007	
0.742 (1 0 0 6 2)			
0.251 (1 0 0 6 4)			
2906.3256	2906.3261	-0.0005	
0.330 (0 0 1 6 1)			
0.614 (0 0 1 6 3)			
2968.3264	2968.3260	0.0004	
0.671 (1 0 0 6 4)			
2980.4496	2980.4490	0.0006	
0.519 (0 0 1 6 1)			
0.354 (0 0 1 6 5)			
3013.9854	3013.9863	-0.0009	
0.535 (0 0 1 6 5)			
3025.6501	3025.6480	0.0021	
0.839 (1 0 0 6 6)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2580.9282	2580.9308	-0.0026	
0.820 (0 2 0 6 1)			
2691.6977	2691.6965	0.0012	
0.652 (0 2 0 6 3)			
2763.8456	2763.8432	0.0024	
0.811 (0 2 0 6 5)			
2838.9746	2838.9741	0.0005	
0.815 (1 0 0 6 1)			
2853.6421	2853.6431	-0.0010	
0.489 (0 0 1 6 0)			
0.466 (0 0 1 6 2)			
2934.7388	2934.7380	0.0008	
0.636 (1 0 0 6 3)			
2948.9352	2948.9354	-0.0002	
0.297 (0 0 1 6 0)			
0.575 (0 0 1 6 4)			
2995.3037	2995.3043	-0.0006	
0.643 (1 0 0 6 5)			
3000.4831	3000.4800	0.0031	
0.318 (0 0 1 6 2)			
3037.7555	3037.7572	-0.0017	
0.884 (0 0 1 6 6)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2723.2820	2723.2827	-0.0007	
0.666 (0 2 0 7 2)			
0.318 (0 2 0 7 4)			
2832.7383	2832.7368	0.0015	
0.307 (0 2 0 7 2)			
0.499 (0 2 0 7 4)			
2908.5914	2908.5893	0.0021	
0.791 (0 2 0 7 6)			
2971.4003	2971.3990	0.0013	
0.655 (1 0 0 7 2)			
0.327 (1 0 0 7 4)			
2986.0726	2986.0725	0.0001	
0.266 (0 0 1 7 1)			
0.629 (0 0 1 7 3)			
3066.2525	3066.2514	0.0011	
0.313 (1 0 0 7 2)			
0.477 (1 0 0 7 4)			
3080.1132	3080.1125	0.0007	
0.423 (0 0 1 7 1)			
0.532 (0 0 1 7 5)			
3125.9746	3125.9756	-0.0010	
0.262 (1 0 0 7 6)			
3132.8024	3132.7998	0.0026	
0.504 (1 0 0 7 6)			
3175.3263	3175.3263	0.0000	
0.887 (0 0 1 7 7)			

SYMMETRY A2				
EIGENSTATE		Eexp	Ecalc	Residual
		2650.9444	2650.9466	-0.0022
0.782	(0 2 0 7 1)			
		2783.7539	2783.7530	0.0009
0.503	(0 2 0 7 3)			
0.302	(0 2 0 7 5)			
		2872.4396	2872.4374	0.0022
0.283	(0 2 0 7 3)			
0.617	(0 2 0 7 5)			
		2908.9444	2908.9443	0.0001
0.776	(1 0 0 7 1)			
		2923.8362	2923.8367	-0.0005
0.453	(0 0 1 7 0)			
0.479	(0 0 1 7 2)			
		2946.9100	2946.9104	-0.0004
0.924	(0 2 0 7 7)			
		3023.7884	3023.7871	0.0013
0.485	(1 0 0 7 3)			
0.315	(1 0 0 7 5)			
		3038.2629	3038.2624	0.0005
0.264	(0 0 1 7 0)			
0.617	(0 0 1 7 4)			
		3100.0823	3100.0818	0.0005
0.285	(1 0 0 7 3)			
0.584	(1 0 0 7 5)			
		3109.8953	3109.8939	0.0014
0.375	(0 0 1 7 2)			
0.287	(0 0 1 7 6)			
		3146.3704	3146.3701	0.0003
0.585	(0 0 1 7 6)			
		3164.0218	3164.0202	0.0016
0.851	(1 0 0 7 7)			

SYMMETRY B1				
EIGENSTATE		Eexp	Ecalc	Residual
		2650.9444	2650.9466	-0.0022
0.461	(0 2 0 7 0)			
0.476	(0 2 0 7 2)			
		2783.6776	2783.6766	0.0010
0.273	(0 2 0 7 0)			
0.608	(0 2 0 7 4)			
		2864.0124	2864.0128	-0.0004
0.408	(0 2 0 7 2)			
		2908.9444	2908.9443	0.0001
0.456	(1 0 0 7 0)			
0.477	(1 0 0 7 2)			
		2910.7634	2910.7614	0.0020
0.707	(0 2 0 7 6)			
		2923.8362	2923.8367	-0.0005
0.774	(0 0 1 7 1)			

	3023.7544	3023.7532	0.0012
0.267 (1 0 0 7 0)			
0.614 (1 0 0 7 4)			
	3038.2807	3038.2801	0.0006
0.474 (0 0 1 7 3)			
0.325 (0 0 1 7 5)			
	3094.6281	3094.6273	0.0008
0.399 (1 0 0 7 2)			
	3113.9276	3113.9274	0.0002
0.292 (0 0 1 7 3)			
0.550 (0 0 1 7 5)			
	3133.8762	3133.8749	0.0013
0.616 (1 0 0 7 6)			
	3175.1682	3175.1682	0.0000
0.897 (0 0 1 7 7)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	2723.2813	2723.2803	0.0010
0.279 (0 2 0 7 1)			
0.625 (0 2 0 7 3)			
	2831.5170	2831.5165	0.0005
0.455 (0 2 0 7 1)			
0.492 (0 2 0 7 5)			
	2885.2279	2885.2275	0.0004
0.262 (0 2 0 7 1)			
0.334 (0 2 0 7 3)			
0.345 (0 2 0 7 5)			
	2947.0190	2947.0192	-0.0002
0.919 (0 2 0 7 7)			
	2971.3993	2971.3982	0.0011
0.271 (1 0 0 7 1)			
0.627 (1 0 0 7 3)			
	2986.0728	2986.0729	-0.0001
0.648 (0 0 1 7 2)			
0.333 (0 0 1 7 4)			
	3065.5957	3065.5948	0.0009
0.437 (1 0 0 7 1)			
0.514 (1 0 0 7 5)			
	3080.5093	3080.5089	0.0004
0.317 (0 0 1 7 2)			
0.460 (0 0 1 7 4)			
	3112.8982	3112.8973	0.0009
0.284 (1 0 0 7 1)			
0.336 (1 0 0 7 3)			
0.299 (1 0 0 7 5)			
	3143.7189	3143.7190	-0.0001
0.706 (0 0 1 7 6)			
	3164.0790	3164.0777	0.0013
0.854 (1 0 0 7 7)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2730.1367	2730.1383	-0.0016	
0.432 (0 2 0 8 0)			
0.483 (0 2 0 8 2)			
2884.9868	2884.9858	0.0010	
0.599 (0 2 0 8 4)			
2988.1880	2988.1876	0.0004	
0.428 (1 0 0 8 0)			
0.484 (1 0 0 8 2)			
2989.9250	2989.9259	-0.0009	
0.315 (0 2 0 8 2)			
0.410 (0 2 0 8 6)			
3003.3371	3003.3372	-0.0001	
0.739 (0 0 1 8 1)			
3042.8612	3042.8617	-0.0005	
0.303 (0 2 0 8 4)			
0.380 (0 2 0 8 6)			
3116.8108	3116.8105	0.0003	
0.920 (0 2 0 8 8)			
3122.0822	3122.0809	0.0013	
0.596 (1 0 0 8 4)			
3136.7740	3136.7731	0.0009	
0.351 (0 0 1 8 3)			
0.415 (0 0 1 8 5)			
3214.1425	3214.1422	0.0003	
0.292 (1 0 0 8 2)			
0.434 (1 0 0 8 6)			
3230.1065	3230.1061	0.0004	
0.365 (0 0 1 8 3)			
0.350 (0 0 1 8 5)			
3260.2718	3260.2713	0.0005	
0.299 (1 0 0 8 4)			
0.314 (1 0 0 8 6)			
3297.0574	3297.0561	0.0013	
0.685 (0 0 1 8 7)			
3321.8424	3321.8412	0.0012	
0.852 (1 0 0 8 8)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
2813.5788	2813.5789	-0.0001	
0.622 (0 2 0 8 3)			
2944.2923	2944.2918	0.0005	
0.368 (0 2 0 8 1)			
0.551 (0 2 0 8 5)			
3019.4842	3019.4858	-0.0016	
0.380 (0 2 0 8 1)			
0.329 (0 2 0 8 3)			
3060.2048	3060.2036	0.0012	
0.622 (1 0 0 8 3)			
3075.1009	3075.1007	0.0002	
0.574 (0 0 1 8 2)			

0.388 (0 0 1 8 4)	3075.1877	3075.1869	0.0008
0.741 (0 2 0 8 7)	3173.7467	3173.7457	0.0010
0.352 (1 0 0 8 1)			
0.554 (1 0 0 8 5)	3188.3874	3188.3863	0.0011
0.349 (0 0 1 8 2)			
0.285 (0 0 1 8 4)			
0.350 (0 0 1 8 6)	3240.6586	3240.6578	0.0008
0.394 (1 0 0 8 1)			
0.316 (1 0 0 8 3)	3264.3751	3264.3740	0.0011
0.299 (0 0 1 8 4)			
0.486 (0 0 1 8 6)	3286.8629	3286.8610	0.0019
0.632 (1 0 0 8 7)	3332.1900	3332.1886	0.0014
0.889 (0 0 1 8 8)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
2813.5792	2813.5793	-0.0001	
0.592 (0 2 0 8 2)			
0.375 (0 2 0 8 4)	2944.6044	2944.6038	0.0006
0.344 (0 2 0 8 2)			
0.323 (0 2 0 8 4)			
0.324 (0 2 0 8 6)	3034.2689	3034.2680	0.0009
0.294 (0 2 0 8 4)			
0.575 (0 2 0 8 6)	3060.2049	3060.2038	0.0011
0.580 (1 0 0 8 2)			
0.383 (1 0 0 8 4)	3075.1008	3075.1006	0.0002
0.621 (0 0 1 8 3)	3116.7634	3116.7634	0.0000
0.923 (0 2 0 8 8)	3173.8881	3173.8871	0.0010
0.348 (1 0 0 8 2)			
0.300 (1 0 0 8 4)			
0.339 (1 0 0 8 6)	3188.3123	3188.3116	0.0007
0.342 (0 0 1 8 1)			
0.557 (0 0 1 8 5)	3250.0447	3250.0447	0.0000
0.257 (1 0 0 8 4)			
0.488 (1 0 0 8 6)	3257.1652	3257.1641	0.0011
0.330 (0 0 1 8 1)			

0.258 (0 0 1 8 3)	3298.5418	3298.5406	0.0012
0.619 (0 0 1 8 7)	3321.8177	3321.8164	0.0013
0.851 (1 0 0 8 8)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2730.1367	2730.1383	-0.0016	
0.748 (0 2 0 8 1)	2885.0023	2885.0016	0.0007
0.379 (0 2 0 8 3)			
0.395 (0 2 0 8 5)	2988.1880	2988.1876	0.0004
0.742 (1 0 0 8 1)	2993.1907	2993.1899	0.0008
0.358 (0 2 0 8 3)			
0.402 (0 2 0 8 5)	3003.3371	3003.3372	-0.0001
0.425 (0 0 1 8 0)			
0.485 (0 0 1 8 2)	3074.0939	3074.0927	0.0012
0.783 (0 2 0 8 7)	3122.0871	3122.0868	0.0003
0.361 (1 0 0 8 3)			
0.407 (1 0 0 8 5)	3136.7714	3136.7704	0.0010
0.594 (0 0 1 8 4)	3215.9578	3215.9571	0.0007
0.363 (1 0 0 8 3)			
0.373 (1 0 0 8 5)	3228.9666	3228.9658	0.0008
0.272 (0 0 1 8 2)			
0.464 (0 0 1 8 6)	3273.6123	3273.6126	-0.0003
0.267 (0 0 1 8 4)	3286.1705	3286.1694	0.0011
0.614 (1 0 0 8 7)	3332.2653	3332.2633	0.0020
0.885 (0 0 1 8 8)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2913.0308	2913.0300	0.0008	
0.530 (0 2 0 9 2)			
0.414 (0 2 0 9 4)	3065.7393	3065.7389	0.0004
0.359 (0 2 0 9 2)			
0.420 (0 2 0 9 6)	3158.2477	3158.2462	0.0015
0.519 (1 0 0 9 2)			
0.420 (1 0 0 9 4)			

	3173.0032	3173.0040	-0.0008
0.364 (0 2 0 9 4)			
0.342 (0 2 0 9 6)			
	3173.4006	3173.4002	0.0004
0.602 (0 0 1 9 3)			
	3260.1580	3260.1577	0.0003
0.779 (0 2 0 9 8)			
	3290.7903	3290.7898	0.0005
0.360 (1 0 0 9 2)			
0.432 (1 0 0 9 6)			
	3305.4834	3305.4827	0.0007
0.286 (0 0 1 9 1)			
0.496 (0 0 1 9 5)			
	3383.7151	3383.7144	0.0007
0.362 (1 0 0 9 4)			
0.308 (1 0 0 9 6)			
	3395.0378	3395.0372	0.0006
0.386 (0 0 1 9 1)			
0.391 (0 0 1 9 7)			
	3439.9532	3439.9526	0.0006
0.267 (0 0 1 9 5)			
0.287 (0 0 1 9 7)			
	3459.2011	3459.2021	-0.0010
0.634 (1 0 0 9 8)			
	3508.2701	3508.2671	0.0030
0.878 (0 0 1 9 9)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	2818.4951	2818.4958	-0.0007
0.718 (0 2 0 9 1)			
0.252 (0 2 0 9 3)			
	2995.3713	2995.3699	0.0014
0.281 (0 2 0 9 3)			
0.454 (0 2 0 9 5)			
	3076.6925	3076.6921	0.0004
0.712 (1 0 0 9 1)			
0.255 (1 0 0 9 3)			
	3092.1326	3092.1329	-0.0003
0.402 (0 0 1 9 0)			
0.486 (0 0 1 9 2)			
	3124.4206	3124.4206	0.0000
0.387 (0 2 0 9 3)			
0.323 (0 2 0 9 7)			
	3216.2700	3216.2706	-0.0006
0.294 (0 2 0 9 5)			
0.551 (0 2 0 9 7)			
	3229.5880	3229.5869	0.0011
0.265 (1 0 0 9 3)			
0.463 (1 0 0 9 5)			
	3244.4952	3244.4947	0.0005
0.542 (0 0 1 9 4)			

	3306.8118	3306.8110	0.0008
0.921 (0 2 0 9 9)			
	3341.9169	3341.9168	0.0001
0.388 (1 0 0 9 3)			
0.338 (1 0 0 9 7)			
	3356.1448	3356.1437	0.0011
0.482 (0 0 1 9 6)			
	3416.6771	3416.6771	0.0000
0.281 (1 0 0 9 7)			
	3423.9812	3423.9815	-0.0003
	3470.3532	3470.3517	0.0015
0.634 (0 0 1 9 8)			
	3498.7460	3498.7451	0.0009
0.846 (1 0 0 9 9)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	2818.4951	2818.4958	-0.0007
0.409 (0 2 0 9 0)			
0.486 (0 2 0 9 2)			
	2995.3680	2995.3666	0.0014
0.555 (0 2 0 9 4)			
	3076.6925	3076.6921	0.0004
0.404 (1 0 0 9 0)			
0.486 (1 0 0 9 2)			
	3092.1326	3092.1329	-0.0003
0.709 (0 0 1 9 1)			
0.257 (0 0 1 9 3)			
	3123.4140	3123.4148	-0.0008
0.476 (0 2 0 9 6)			
	3193.5583	3193.5612	-0.0029
0.293 (0 2 0 9 2)			
0.290 (0 2 0 9 4)			
	3229.5869	3229.5858	0.0011
0.547 (1 0 0 9 4)			
	3244.4958	3244.4951	0.0007
0.256 (0 0 1 9 3)			
0.468 (0 0 1 9 5)			
	3260.6797	3260.6804	-0.0007
0.760 (0 2 0 9 8)			
	3341.4478	3341.4471	0.0007
0.479 (1 0 0 9 6)			
	3356.3997	3356.3992	0.0005
0.387 (0 0 1 9 3)			
0.346 (0 0 1 9 7)			
	3404.1320	3404.1315	0.0005
0.308 (1 0 0 9 2)			
0.273 (1 0 0 9 4)			
	3433.6545	3433.6530	0.0015
0.295 (0 0 1 9 5)			
0.445 (0 0 1 9 7)			
	3459.5561	3459.5563	-0.0002

0.637 (1 0 0 9 8)	3508.2357	3508.2320	0.0037
0.880 (0 0 1 9 9)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
2913.0307	2913.0299	0.0008	
0.607 (0 2 0 9 3)	3065.6641	3065.6640	0.0001
0.305 (0 2 0 9 1)			
0.511 (0 2 0 9 5)	3158.2477	3158.2462	0.0015
0.603 (1 0 0 9 3)	3165.8315	3165.8338	-0.0023
0.415 (0 2 0 9 1)			
0.327 (0 2 0 9 7)	3173.4006	3173.4001	0.0005
0.513 (0 0 1 9 2)			
0.424 (0 0 1 9 4)	3221.4519	3221.4531	-0.0012
0.290 (0 2 0 9 5)			
0.429 (0 2 0 9 7)	3290.7620	3290.7611	0.0009
0.293 (1 0 0 9 1)			
0.502 (1 0 0 9 5)	3305.4968	3305.4961	0.0007
0.360 (0 0 1 9 2)			
0.440 (0 0 1 9 6)	3306.8323	3306.8315	0.0008
0.920 (0 2 0 9 9)	3379.5810	3379.5809	0.0001
0.411 (1 0 0 9 1)			
0.344 (1 0 0 9 7)	3397.7803	3397.7801	0.0002
0.362 (0 0 1 9 4)			
0.279 (0 0 1 9 6)	3427.0790	3427.0783	0.0007
0.283 (1 0 0 9 5)			
0.340 (1 0 0 9 7)	3469.5724	3469.5705	0.0019
0.667 (0 0 1 9 8)	3498.7563	3498.7551	0.0012
0.846 (1 0 0 9 9)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
2916.0075	2916.0075	0.0000	
0.389 (0 2 0 10 0)			
0.485 (0 2 0 10 2)	3114.8383	3114.8384	-0.0001
0.499 (0 2 0 10 4)			
0.267 (0 2 0 10 6)			

	3174.4429	3174.4443	-0.0014
0.384 (1 0 0 10 0)			
0.485 (1 0 0 10 2)			
	3190.2110	3190.2100	0.0010
0.682 (0 0 1 10 1)			
0.273 (0 0 1 10 3)			
	3264.8574	3264.8584	-0.0010
0.420 (0 2 0 10 6)			
	3346.2682	3346.2678	0.0004
0.486 (1 0 0 10 4)			
0.278 (1 0 0 10 6)			
	3358.8796	3358.8825	-0.0029
0.335 (0 2 0 10 2)			
0.260 (0 2 0 10 8)			
	3361.4321	3361.4316	0.0005
0.490 (0 0 1 10 5)			
	3421.2549	3421.2574	-0.0025
0.286 (0 2 0 10 6)			
0.471 (0 2 0 10 8)			
	3477.1320	3477.1318	0.0002
0.406 (1 0 0 10 6)			
	3491.9713	3491.9705	0.0008
0.372 (0 0 1 10 3)			
0.432 (0 0 1 10 7)			
	3516.6197	3516.6187	0.0010
0.917 (0 2 0 10 10)			
	3561.4559	3561.4556	0.0003
0.333 (1 0 0 10 2)			
0.261 (1 0 0 10 8)			
	3583.6083	3583.6076	0.0007
0.342 (0 0 1 10 5)			
	3613.6227	3613.6229	-0.0002
0.274 (1 0 0 10 6)			
0.361 (1 0 0 10 8)			
	3661.0958	3661.0936	0.0022
0.650 (0 0 1 10 9)			
	3694.5055	3694.5052	0.0003
0.838 (1 0 0 10 10)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	3021.6260	3021.6255	0.0005
0.585 (0 2 0 10 3)			
	3195.9296	3195.9295	0.0001
0.260 (0 2 0 10 1)			
0.431 (0 2 0 10 5)			
	3265.5134	3265.5125	0.0009
0.580 (1 0 0 10 3)			
	3280.9578	3280.9572	0.0006
0.461 (0 0 1 10 2)			
0.447 (0 0 1 10 4)			
	3320.2914	3320.2927	-0.0013

0.373 (0 2 0 10 1)			
0.399 (0 2 0 10 7)			
	3386.9135	3386.9152	-0.0017
0.280 (0 2 0 10 5)			
	3416.8268	3416.8269	-0.0001
0.250 (1 0 0 10 1)			
0.414 (1 0 0 10 5)			
0.261 (1 0 0 10 7)			
	3431.7619	3431.7609	0.0010
0.358 (0 0 1 10 2)			
0.477 (0 0 1 10 6)			
	3466.7306	3466.7321	-0.0015
0.767 (0 2 0 10 9)			
	3526.3534	3526.3532	0.0002
0.356 (1 0 0 10 1)			
0.402 (1 0 0 10 7)			
	3542.0823	3542.0833	-0.0010
0.366 (0 0 1 10 4)			
0.325 (0 0 1 10 8)			
	3585.5702	3585.5696	0.0006
0.255 (1 0 0 10 5)			
	3621.7616	3621.7589	0.0027
0.288 (0 0 1 10 6)			
0.417 (0 0 1 10 8)			
	3651.6044	3651.6066	-0.0022
0.632 (1 0 0 10 9)			
	3703.0149	3703.0119	0.0030
0.869 (0 0 1 10 10)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	3021.6260	3021.6255	0.0005
0.478 (0 2 0 10 2)			
0.440 (0 2 0 10 4)			
	3195.9472	3195.9472	0.0000
0.360 (0 2 0 10 2)			
0.468 (0 2 0 10 6)			
	3265.5134	3265.5125	0.0009
0.467 (1 0 0 10 2)			
0.444 (1 0 0 10 4)			
	3280.9578	3280.9572	0.0006
0.577 (0 0 1 10 3)			
	3322.9840	3322.9846	-0.0006
0.376 (0 2 0 10 4)			
0.312 (0 2 0 10 8)			
	3416.8314	3416.8299	0.0015
0.359 (1 0 0 10 2)			
0.471 (1 0 0 10 6)			
	3418.4174	3418.4220	-0.0046
0.289 (0 2 0 10 6)			
0.538 (0 2 0 10 8)			
	3431.7596	3431.7585	0.0011

0.405 (0 0 1 10 5)			
0.270 (0 0 1 10 7)			
	3516.6109	3516.6096	0.0013
0.918 (0 2 0 10 10)			
	3527.6627	3527.6635	-0.0008
0.371 (1 0 0 10 4)			
0.324 (1 0 0 10 8)			
	3541.3383	3541.3378	0.0005
0.338 (0 0 1 10 1)			
0.411 (0 0 1 10 7)			
	3599.1640	3599.1654	-0.0014
	3611.5393	3611.5410	-0.0017
0.346 (1 0 0 10 8)			
	3661.4912	3661.4892	0.0020
0.634 (0 0 1 10 9)			
	3694.5026	3694.5014	0.0012
0.837 (1 0 0 10 10)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	2916.0075	2916.0075	0.0000
0.692 (0 2 0 10 1)			
0.268 (0 2 0 10 3)			
	3114.8390	3114.8391	-0.0001
0.483 (0 2 0 10 5)			
	3174.4429	3174.4443	-0.0014
0.685 (1 0 0 10 1)			
0.271 (1 0 0 10 3)			
	3190.2101	3190.2100	0.0001
0.382 (0 0 1 10 0)			
0.485 (0 0 1 10 2)			
	3265.1366	3265.1371	-0.0005
0.380 (0 2 0 10 3)			
0.414 (0 2 0 10 7)			
	3346.2684	3346.2681	0.0003
0.488 (1 0 0 10 5)			
	3361.4320	3361.4314	0.0006
0.480 (0 0 1 10 4)			
0.285 (0 0 1 10 6)			
	3372.1941	3372.1951	-0.0010
0.355 (0 2 0 10 5)			
0.308 (0 2 0 10 7)			
	3466.4876	3466.4896	-0.0020
0.776 (0 2 0 10 9)			
	3477.2416	3477.2420	-0.0004
0.376 (1 0 0 10 3)			
0.425 (1 0 0 10 7)			
	3491.9187	3491.9178	0.0009
0.396 (0 0 1 10 6)			
	3569.2274	3569.2274	0.0000
0.327 (1 0 0 10 5)			
0.260 (1 0 0 10 7)			

	3578.1639	3578.1648	-0.0009
0.285 (0 0 1 10 2)			
0.328 (0 0 1 10 8)			
	3625.6428	3625.6432	-0.0004
0.268 (0 0 1 10 6)			
0.322 (0 0 1 10 8)			
	3651.4374	3651.4396	-0.0022
0.631 (1 0 0 10 9)			
	3703.0313	3703.0285	0.0028
0.869 (0 0 1 10 10)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	3139.3567	3139.3555	0.0012
0.434 (0 2 0 11 2)			
0.455 (0 2 0 11 4)			
	3335.1773	3335.1772	0.0001
0.353 (0 2 0 11 2)			
0.474 (0 2 0 11 6)			
	3381.9870	3381.9869	0.0001
0.423 (1 0 0 11 2)			
0.458 (1 0 0 11 4)			
	3397.7570	3397.7565	0.0005
0.551 (0 0 1 11 3)			
0.268 (0 0 1 11 5)			
	3482.8579	3482.8586	-0.0007
0.344 (0 2 0 11 4)			
0.395 (0 2 0 11 8)			
	3551.9803	3551.9800	0.0003
0.351 (1 0 0 11 2)			
0.473 (1 0 0 11 6)			
	3567.1578	3567.1596	-0.0018
0.313 (0 0 1 11 5)			
0.338 (0 0 1 11 7)			
	3590.8036	3590.8039	-0.0003
0.345 (0 2 0 11 6)			
0.288 (0 2 0 11 8)			
	3681.1673	3681.1674	-0.0001
0.332 (1 0 0 11 4)			
0.401 (1 0 0 11 8)			
	3692.7184	3692.7206	-0.0022
0.772 (0 2 0 11 10)			
	3695.7346	3695.7316	0.0030
0.286 (0 0 1 11 1)			
0.315 (0 0 1 11 7)			
	3771.3984	3771.3986	-0.0002
	3779.3335	3779.3369	-0.0034
0.259 (0 0 1 11 9)			
	3830.8349	3830.8354	-0.0005
0.270 (0 0 1 11 7)			
0.344 (0 0 1 11 9)			
	3862.5649	3862.5686	-0.0037

0.619 (1 0 0 11 10)	3916.2278	3916.2315	-0.0037
0.855 (0 0 1 11 11)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
3022.6605	3022.6608	-0.0003	
0.669 (0 2 0 11 1)			
0.280 (0 2 0 11 3)			
3243.3988	3243.3991	-0.0003	
0.491 (0 2 0 11 5)			
3281.4281	3281.4292	-0.0011	
0.662 (1 0 0 11 1)			
0.283 (1 0 0 11 3)			
3297.5538	3297.5537	0.0001	
0.366 (0 0 1 11 0)			
0.482 (0 0 1 11 2)			
3414.9212	3414.9215	-0.0003	
0.354 (0 2 0 11 3)			
0.447 (0 2 0 11 7)			
3472.1152	3472.1149	0.0003	
0.491 (1 0 0 11 5)			
3487.5673	3487.5672	0.0001	
0.419 (0 0 1 11 4)			
0.333 (0 0 1 11 6)			
3540.1679	3540.1678	0.0001	
0.352 (0 2 0 11 5)			
0.299 (0 2 0 11 9)			
3621.6578	3621.6583	-0.0005	
0.346 (1 0 0 11 3)			
0.448 (1 0 0 11 7)			
3636.6035	3636.6055	-0.0020	
0.283 (0 0 1 11 6)			
0.295 (0 0 1 11 8)			
3640.5889	3640.5894	-0.0005	
0.288 (0 2 0 11 7)			
0.531 (0 2 0 11 9)			
3730.9271	3730.9273	-0.0002	
0.339 (1 0 0 11 5)			
0.306 (1 0 0 11 9)			
3743.3891	3743.3900	-0.0009	
0.254 (0 0 1 11 2)			
0.348 (0 0 1 11 8)			
3745.6937	3745.6934	0.0003	
0.914 (0 2 0 11 11)			
3799.1405	3799.1435	-0.0030	
3818.6729	3818.6754	-0.0025	
0.258 (1 0 0 11 7)			
0.371 (1 0 0 11 9)			
3871.5938	3871.5937	0.0001	
0.624 (0 0 1 11 10)			
3908.7656	3908.7652	0.0004	

0.825 (1 0 0 11 11)

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
3022.6605	3022.6608	-0.0003	
0.373 (0 2 0 11 0)			
0.483 (0 2 0 11 2)			
3243.3987	3243.3989	-0.0002	
0.440 (0 2 0 11 4)			
0.317 (0 2 0 11 6)			
3281.4281	3281.4292	-0.0011	
0.368 (1 0 0 11 0)			
0.482 (1 0 0 11 2)			
3297.5538	3297.5537	0.0001	
0.659 (0 0 1 11 1)			
0.285 (0 0 1 11 3)			
3414.8471	3414.8471	0.0000	
0.318 (0 2 0 11 6)			
0.269 (0 2 0 11 8)			
3472.1152	3472.1149	0.0003	
0.426 (1 0 0 11 4)			
0.327 (1 0 0 11 6)			
3487.5673	3487.5673	0.0000	
0.491 (0 0 1 11 5)			
3534.0556	3534.0560	-0.0004	
0.299 (0 2 0 11 2)			
0.327 (0 2 0 11 8)			
3600.3356	3600.3342	0.0014	
0.287 (0 2 0 11 6)			
3621.6337	3621.6344	-0.0007	
0.296 (1 0 0 11 6)			
0.284 (1 0 0 11 8)			
3636.6167	3636.6163	0.0004	
0.340 (0 0 1 11 3)			
0.449 (0 0 1 11 7)			
3692.8296	3692.8296	0.0000	
0.768 (0 2 0 11 10)			
3727.8002	3727.8006	-0.0004	
0.280 (1 0 0 11 2)			
0.326 (1 0 0 11 8)			
3745.2796	3745.2817	-0.0021	
0.330 (0 0 1 11 5)			
0.291 (0 0 1 11 9)			
3785.6261	3785.6257	0.0004	
0.254 (1 0 0 11 6)			
3828.6296	3828.6292	0.0004	
0.282 (0 0 1 11 7)			
0.397 (0 0 1 11 9)			
3862.6403	3862.6439	-0.0036	
0.620 (1 0 0 11 10)			
3916.2198	3916.2235	-0.0037	
0.856 (0 0 1 11 11)			

SYMMETRY B2				
EIGENSTATE		Eexp	Ecalc	Residual
		3139.3567	3139.3555	0.0012
0.561	(0 2 0 11 3)			
0.257	(0 2 0 11 5)			
		3335.1733	3335.1729	0.0004
0.343	(0 2 0 11 5)			
0.318	(0 2 0 11 7)			
		3381.9870	3381.9869	0.0001
0.554	(1 0 0 11 3)			
0.264	(1 0 0 11 5)			
		3397.7570	3397.7565	0.0005
0.418	(0 0 1 11 2)			
0.460	(0 0 1 11 4)			
		3481.9931	3481.9937	-0.0006
0.315	(0 2 0 11 1)			
0.343	(0 2 0 11 7)			
		3551.9791	3551.9787	0.0004
0.323	(1 0 0 11 5)			
0.330	(1 0 0 11 7)			
		3567.1580	3567.1597	-0.0017
0.349	(0 0 1 11 2)			
0.472	(0 0 1 11 6)			
		3569.2999	3569.2965	0.0034
0.292	(0 2 0 11 1)			
0.277	(0 2 0 11 3)			
		3642.0340	3642.0357	-0.0017
0.286	(0 2 0 11 7)			
0.497	(0 2 0 11 9)			
		3680.8145	3680.8150	-0.0005
0.298	(1 0 0 11 1)			
0.325	(1 0 0 11 7)			
		3695.9075	3695.9081	-0.0006
0.323	(0 0 1 11 4)			
0.405	(0 0 1 11 8)			
		3745.6970	3745.6966	0.0004
0.914	(0 2 0 11 11)			
		3759.7606	3759.7608	-0.0002
0.311	(1 0 0 11 1)			
0.274	(1 0 0 11 3)			
		3787.6926	3787.6940	-0.0014
0.319	(0 0 1 11 6)			
		3819.8213	3819.8217	-0.0004
0.270	(1 0 0 11 7)			
0.371	(1 0 0 11 9)			
		3871.3983	3871.3978	0.0005
0.631	(0 0 1 11 10)			
		3908.7668	3908.7665	0.0003
0.826	(1 0 0 11 11)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
3138.4423	3138.4416	0.0007	
0.358 (0 2 0 12 0)			
0.480 (0 2 0 12 2)			
3381.0390	3381.0394	-0.0004	
0.385 (0 2 0 12 4)			
0.355 (0 2 0 12 6)			
3397.6289	3397.6303	-0.0014	
0.353 (1 0 0 12 0)			
0.478 (1 0 0 12 2)			
3414.1482	3414.1478	0.0004	
0.638 (0 0 1 12 1)			
0.294 (0 0 1 12 3)			
3573.6198	3573.6191	0.0007	
0.341 (0 2 0 12 8)			
3607.1101	3607.1098	0.0003	
0.369 (1 0 0 12 4)			
0.363 (1 0 0 12 6)			
3622.8848	3622.8852	-0.0004	
0.478 (0 0 1 12 5)			
3716.3183	3716.3186	-0.0003	
0.282 (0 2 0 12 8)			
3775.0820	3775.0834	-0.0014	
0.352 (1 0 0 12 8)			
3790.2942	3790.2947	-0.0005	
0.302 (0 0 1 12 3)			
0.416 (0 0 1 12 7)			
0.0000	3797.7596	0.0000	
3883.2514	3883.2468	0.0046	
0.286 (0 2 0 12 8)			
0.508 (0 2 0 12 10)			
3901.3148	3901.3170	-0.0022	
0.262 (1 0 0 12 8)			
3917.0225	3917.0239	-0.0014	
0.266 (0 0 1 12 5)			
0.368 (0 0 1 12 9)			
3974.9501	3974.9502	-0.0001	
3993.5790	3993.5800	-0.0010	
0.909 (0 2 0 12 12)			
4010.0732	4010.0760	-0.0028	
0.301 (0 0 1 12 7)			
4045.3159	4045.3176	-0.0017	
0.266 (1 0 0 12 8)			
0.370 (1 0 0 12 10)			
4100.2047	4100.2088	-0.0041	
0.608 (0 0 1 12 11)			
4141.2087	4141.2071	0.0016	
0.810 (1 0 0 12 12)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
3266.2093	3266.2080	0.0013	

0.536 (0 2 0 12 3)			
0.284 (0 2 0 12 5)			
	3483.4107	3483.4113	-0.0006
0.263 (0 2 0 12 5)			
0.368 (0 2 0 12 7)			
	3507.6526	3507.6521	0.0005
0.527 (1 0 0 12 3)			
0.291 (1 0 0 12 5)			
	3523.7810	3523.7807	0.0003
0.381 (0 0 1 12 2)			
0.465 (0 0 1 12 4)			
	3651.6397	3651.6387	0.0010
0.269 (0 2 0 12 1)			
0.274 (0 2 0 12 9)			
	3696.2120	3696.2134	-0.0014
0.377 (1 0 0 12 7)			
	3711.6783	3711.6785	-0.0002
0.337 (0 0 1 12 2)			
0.441 (0 0 1 12 6)			
	3764.0326	3764.0307	0.0019
0.338 (0 2 0 12 1)			
0.268 (0 2 0 12 9)			
	0.0000	3834.4183	0.0000
0.300 (0 2 0 12 7)			
	3843.6760	3843.6787	-0.0027
0.254 (1 0 0 12 1)			
0.289 (1 0 0 12 9)			
	3858.7595	3858.7589	0.0006
0.262 (0 0 1 12 4)			
0.405 (0 0 1 12 8)			
	0.0000	3938.4695	0.0000
0.764 (0 2 0 12 11)			
	3945.0960	3945.0994	-0.0034
0.340 (1 0 0 12 1)			
0.255 (1 0 0 12 9)			
	3965.9876	3965.9912	-0.0036
0.292 (0 0 1 12 6)			
0.253 (0 0 1 12 10)			
	4004.8878	4004.8874	0.0004
0.259 (1 0 0 12 7)			
	4054.1415	4054.1414	0.0001
0.277 (0 0 1 12 8)			
0.379 (0 0 1 12 10)			
	4092.2969	4092.3008	-0.0039
0.601 (1 0 0 12 11)			
	0.0000	4147.5531	0.0000
0.838 (0 0 1 12 12)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	3266.2091	3266.2080	0.0011
0.397 (0 2 0 12 2)			

0.463 (0 2 0 12 4)	3483.4118	3483.4124	-0.0006
0.343 (0 2 0 12 2)			
0.453 (0 2 0 12 6)	3507.6526	3507.6521	0.0005
0.386 (1 0 0 12 2)			
0.465 (1 0 0 12 4)	3523.7810	3523.7807	0.0003
0.524 (0 0 1 12 3)			
0.295 (0 0 1 12 5)	3651.8996	3651.8985	0.0011
0.289 (0 2 0 12 4)			
0.412 (0 2 0 12 8)	3696.2122	3696.2137	-0.0015
0.340 (1 0 0 12 2)			
0.445 (1 0 0 12 6)	3711.6783	3711.6784	-0.0001
0.383 (0 0 1 12 7)	3775.9381	3775.9357	0.0024
0.329 (0 2 0 12 6)			
0.289 (0 2 0 12 10)	3843.7641	3843.7651	-0.0010
0.273 (1 0 0 12 4)			
0.407 (1 0 0 12 8)	3858.7182	3858.7186	-0.0004
0.301 (0 0 1 12 9)	3882.5488	3882.5451	0.0037
0.288 (0 2 0 12 8)			
0.524 (0 2 0 12 10)	3951.4345	3951.4347	-0.0002
0.301 (1 0 0 12 6)			
0.287 (1 0 0 12 10)	3961.8925	3961.8937	-0.0012
0.300 (0 0 1 12 1)			
0.297 (0 0 1 12 9)	3993.5772	3993.5781	-0.0009
0.909 (0 2 0 12 12)	4017.6871	4017.6914	-0.0043
	4044.7372	4044.7398	-0.0026
0.262 (1 0 0 12 8)			
0.371 (1 0 0 12 10)	4100.3013	4100.3049	-0.0036
0.604 (0 0 1 12 11)	4141.2083	4141.2067	0.0016
0.810 (1 0 0 12 12)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	3138.4423	3138.4416	0.0007
0.648 (0 2 0 12 1)			
0.290 (0 2 0 12 3)	3381.0390	3381.0394	-0.0004

0.483 (0 2 0 12 5)	3397.6289	3397.6303	-0.0014
0.640 (1 0 0 12 1)			
0.293 (1 0 0 12 3)	3414.1482	3414.1478	0.0004
0.351 (0 0 1 12 0)			
0.477 (0 0 1 12 2)	3573.6395	3573.6389	0.0006
0.319 (0 2 0 12 3)			
0.429 (0 2 0 12 7)	3607.1101	3607.1098	0.0003
0.479 (1 0 0 12 5)	3622.8848	3622.8852	-0.0004
0.362 (0 0 1 12 4)			
0.368 (0 0 1 12 6)	3718.6243	3718.6229	0.0014
0.299 (0 2 0 12 5)			
0.371 (0 2 0 12 9)	3775.0876	3775.0895	-0.0019
0.309 (1 0 0 12 3)			
0.420 (1 0 0 12 7)	3790.2926	3790.2928	-0.0002
0.360 (0 0 1 12 8)	3828.8478	3828.8438	0.0040
0.337 (0 2 0 12 7)			
0.277 (0 2 0 12 9)	3902.3043	3902.3053	-0.0010
0.280 (1 0 0 12 5)			
0.372 (1 0 0 12 9)	3916.5020	3916.5023	-0.0003
0.253 (0 0 1 12 8)	0.0000	3938.4249	0.0000
0.767 (0 2 0 12 11)	3988.6519	3988.6528	-0.0009
	4000.4041	4000.4080	-0.0039
	4055.3204	4055.3228	-0.0024
0.270 (0 0 1 12 8)			
0.352 (0 0 1 12 10)	4092.2637	4092.2678	-0.0041
0.601 (1 0 0 12 11)	0.0000	4147.5570	0.0000
0.838 (0 0 1 12 12)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
3402.1712	3402.1699	0.0013	
0.366 (0 2 0 13 2)			
0.466 (0 2 0 13 4)	3640.6410	3640.6398	0.0012
0.330 (0 2 0 13 2)			
0.415 (0 2 0 13 6)	3642.4902	3642.4899	0.0003

0.354 (1 0 0 13 2)			
0.465 (1 0 0 13 4)			
	3659.0120	3659.0123	-0.0003
0.498 (0 0 1 13 3)			
0.316 (0 0 1 13 5)			
	3829.8096	3829.8080	0.0016
0.374 (0 2 0 13 8)			
	3849.5134	3849.5147	-0.0013
0.327 (1 0 0 13 2)			
0.402 (1 0 0 13 6)			
	3865.2991	3865.2988	0.0003
0.405 (0 0 1 13 7)			
	3972.2433	3972.2422	0.0011
0.254 (0 2 0 13 4)			
0.262 (0 2 0 13 6)			
0.348 (0 2 0 13 10)			
	4015.2828	4015.2853	-0.0025
0.358 (1 0 0 13 8)			
	4030.5142	4030.5176	-0.0034
0.262 (0 0 1 13 5)			
0.360 (0 0 1 13 9)			
	0.0000	4086.2494	0.0000
0.332 (0 2 0 13 8)			
0.269 (0 2 0 13 10)			
	4140.4050	4140.4060	-0.0010
0.258 (1 0 0 13 4)			
0.344 (1 0 0 13 10)			
	0.0000	4153.7126	0.0000
0.287 (0 0 1 13 1)			
	4203.1424	4203.1468	-0.0044
0.759 (0 2 0 13 12)			
	0.0000	4221.9538	0.0000
	4240.9449	4240.9479	-0.0030
0.255 (1 0 0 13 8)			
	0.0000	4298.7181	0.0000
0.270 (0 0 1 13 9)			
0.347 (0 0 1 13 11)			
	4340.1884	4340.1917	-0.0033
0.576 (1 0 0 13 12)			
	0.0000	4396.6882	0.0000
0.817 (0 0 1 13 13)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	3263.3353	3263.3345	0.0008
0.630 (0 2 0 13 1)			
0.298 (0 2 0 13 3)			
	3523.0273	3523.0297	-0.0024
0.621 (1 0 0 13 1)			
0.300 (1 0 0 13 3)			
	3527.7463	3527.7472	-0.0009
0.466 (0 2 0 13 5)			

	3539.9739	3539.9752	-0.0013
0.338 (0 0 1 13 0)			
0.472 (0 0 1 13 2)			
	3741.2519	3741.2494	0.0025
0.283 (0 2 0 13 3)			
0.381 (0 2 0 13 7)			
	3751.2328	3751.2334	-0.0006
0.459 (1 0 0 13 5)			
	3767.3662	3767.3666	-0.0004
0.311 (0 0 1 13 4)			
0.390 (0 0 1 13 6)			
	3906.5030	3906.5036	-0.0006
0.256 (0 2 0 13 3)			
0.374 (0 2 0 13 9)			
	3937.5049	3937.5065	-0.0016
0.271 (1 0 0 13 3)			
0.364 (1 0 0 13 7)			
	3952.9914	3952.9902	0.0012
0.393 (0 0 1 13 8)			
	0.0000	4030.3165	0.0000
0.313 (0 2 0 13 7)			
0.283 (0 2 0 13 11)			
	4082.8426	4082.8440	-0.0014
0.259 (1 0 0 13 3)			
0.364 (1 0 0 13 9)			
	4097.7380	4097.7366	0.0014
0.295 (0 0 1 13 10)			
	0.0000	4143.9530	0.0000
0.289 (0 2 0 13 9)			
0.516 (0 2 0 13 11)			
	4188.3885	4188.3868	0.0017
	0.0000	4197.2131	0.0000
	4255.3317	4255.3299	0.0018
	4259.7744	4259.7761	-0.0017
0.901 (0 2 0 13 13)			
	0.0000	4289.3932	0.0000
0.262 (1 0 0 13 9)			
0.360 (1 0 0 13 11)			
	0.0000	4347.2666	0.0000
0.578 (0 0 1 13 12)			
	4391.4928	4391.4935	-0.0007
0.791 (1 0 0 13 13)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	3263.3353	3263.3345	0.0008
0.346 (0 2 0 13 0)			
0.476 (0 2 0 13 2)			
	3523.0273	3523.0297	-0.0024
0.340 (1 0 0 13 0)			
0.473 (1 0 0 13 2)			
	3527.7463	3527.7472	-0.0009

0.335 (0 2 0 13 4)			
0.381 (0 2 0 13 6)			
	3539.9739	3539.9752	-0.0013
0.618 (0 0 1 13 1)			
0.301 (0 0 1 13 3)			
	3741.2466	3741.2441	0.0025
0.383 (0 2 0 13 8)			
	3751.2328	3751.2333	-0.0005
0.318 (1 0 0 13 4)			
0.387 (1 0 0 13 6)			
	3767.3662	3767.3666	-0.0004
0.456 (0 0 1 13 5)			
	3905.7217	3905.7226	-0.0009
0.267 (0 2 0 13 10)			
	3937.5035	3937.5051	-0.0016
0.389 (1 0 0 13 8)			
	3952.9914	3952.9906	0.0008
0.265 (0 0 1 13 3)			
0.356 (0 0 1 13 7)			
	4010.1458	4010.1434	0.0024
0.278 (0 2 0 13 2)			
	4082.5573	4082.5494	0.0079
0.280 (1 0 0 13 10)			
	4089.2556	4089.2598	-0.0042
0.310 (0 2 0 13 8)			
	4097.8810	4097.8701	0.0109
0.260 (0 0 1 13 3)			
0.358 (0 0 1 13 9)			
	4177.8759	4177.8778	-0.0019
0.285 (1 0 0 13 2)			
	4203.1654	4203.1604	0.0050
0.750 (0 2 0 13 12)			
	4204.3547	4204.3309	0.0238
0.258 (0 0 1 13 7)			
	4243.5910	4243.5897	0.0013
0.263 (1 0 0 13 8)			
	4298.1088	4298.1094	-0.0006
0.273 (0 0 1 13 9)			
0.359 (0 0 1 13 11)			
	4340.2033	4340.2059	-0.0026
0.576 (1 0 0 13 12)			
	0.0000	4396.6862	0.0000
0.817 (0 0 1 13 13)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	3402.1712	3402.1699	0.0013
0.511 (0 2 0 13 3)			
0.306 (0 2 0 13 5)			
	3640.6407	3640.6395	0.0012
0.397 (0 2 0 13 7)			
	3642.4902	3642.4899	0.0003

0.502 (1 0 0 13 3)			
0.313 (1 0 0 13 5)			
	3659.0120	3659.0123	-0.0003
0.350 (0 0 1 13 2)			
0.465 (0 0 1 13 4)			
	3829.7336	3829.7317	0.0019
0.344 (0 2 0 13 9)			
	3849.5134	3849.5147	-0.0013
0.402 (1 0 0 13 7)			
	3865.2991	3865.2988	0.0003
0.324 (0 0 1 13 2)			
0.396 (0 0 1 13 6)			
	3966.9054	3966.9074	-0.0020
0.324 (0 2 0 13 1)			
	4015.2614	4015.2616	-0.0002
0.258 (1 0 0 13 5)			
0.353 (1 0 0 13 9)			
	4030.5216	4030.5261	-0.0045
0.350 (0 0 1 13 8)			
	0.0000	4045.2047	0.0000
	4137.9597	4137.9499	0.0098
0.309 (1 0 0 13 1)			
	4144.2992	4144.3012	-0.0020
0.286 (0 2 0 13 9)			
0.508 (0 2 0 13 11)			
	4155.0935	4155.0890	0.0045
0.262 (0 0 1 13 4)			
0.323 (0 0 1 13 10)			
	4207.7573	4207.7591	-0.0018
	4250.7165	4250.7187	-0.0022
0.288 (0 0 1 13 8)			
	4259.7752	4259.7734	0.0018
0.902 (0 2 0 13 13)			
	4289.6720	4289.6706	0.0014
0.264 (1 0 0 13 9)			
0.360 (1 0 0 13 11)			
	0.0000	4347.2196	0.0000
0.580 (0 0 1 13 12)			
	4391.4928	4391.4936	-0.0008
0.791 (1 0 0 13 13)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	3397.3235	3397.3229	0.0006
0.334 (0 2 0 14 0)			
0.471 (0 2 0 14 2)			
	3657.6057	3657.6084	-0.0027
0.328 (1 0 0 14 0)			
0.468 (1 0 0 14 2)			
	3675.0092	3675.0086	0.0006
0.601 (0 0 1 14 1)			
0.307 (0 0 1 14 3)			

	3683.5131	3683.5167	-0.0036
0.290 (0 2 0 14 4)			
0.397 (0 2 0 14 6)			
	3904.4637	3904.4631	0.0006
0.273 (1 0 0 14 4)			
0.401 (1 0 0 14 6)			
	3917.7097	3917.7083	0.0014
0.392 (0 2 0 14 8)			
	3921.0196	3921.0190	0.0006
0.426 (0 0 1 14 5)			
0.254 (0 0 1 14 7)			
	0.0000	4103.0131	0.0000
0.259 (0 2 0 14 6)			
0.333 (0 2 0 14 10)			
	4108.8872	4108.8917	-0.0045
0.255 (1 0 0 14 4)			
0.395 (1 0 0 14 8)			
	4124.6822	4124.6888	-0.0066
0.287 (0 0 1 14 7)			
0.287 (0 0 1 14 9)			
	0.0000	4232.8763	0.0000
0.277 (0 2 0 14 2)			
	4272.1617	4272.1602	0.0015
0.268 (1 0 0 14 6)			
0.339 (1 0 0 14 10)			
	4287.5251	4287.5267	-0.0016
0.260 (0 0 1 14 3)			
0.288 (0 0 1 14 9)			
	0.0000	4312.5315	0.0000
	0.0000	4389.9470	0.0000
0.264 (1 0 0 14 2)			
	4409.9943	4410.0176	-0.0233
0.256 (0 0 1 14 5)			
0.275 (0 0 1 14 11)			
	0.0000	4424.5610	0.0000
0.290 (0 2 0 14 10)			
0.501 (0 2 0 14 12)			
	0.0000	4458.9944	0.0000
	0.0000	4509.5484	0.0000
0.277 (0 0 1 14 9)			
	0.0000	4543.7349	0.0000
0.891 (0 2 0 14 14)			
	0.0000	4552.4660	0.0000
0.260 (1 0 0 14 10)			
0.343 (1 0 0 14 12)			
	0.0000	4612.1003	0.0000
0.547 (0 0 1 14 13)			
	4659.2968	4659.2970	-0.0002
0.766 (1 0 0 14 14)			

SYMMETRY A2

EIGENSTATE

Eexp

Ecalc

Residual

	3547.2293	3547.2269	0.0024
0.488 (0 2 0 14 3)			
0.324 (0 2 0 14 5)			
	3786.4795	3786.4780	0.0015
0.477 (1 0 0 14 3)			
0.330 (1 0 0 14 5)			
	3803.4062	3803.4025	0.0037
0.320 (0 0 1 14 2)			
0.459 (0 0 1 14 4)			
	3806.8735	3806.8771	-0.0036
0.406 (0 2 0 14 7)			
	4011.8591	4011.8588	0.0003
0.409 (1 0 0 14 7)			
	4016.4601	4016.4633	-0.0032
0.269 (0 2 0 14 5)			
0.374 (0 2 0 14 9)			
	4028.0103	4028.0067	0.0036
0.310 (0 0 1 14 2)			
0.345 (0 0 1 14 6)			
0.289 (0 0 1 14 8)			
	0.0000	4176.3544	0.0000
0.283 (0 2 0 14 1)			
	4195.6684	4195.6695	-0.0011
0.275 (1 0 0 14 5)			
0.375 (1 0 0 14 9)			
	4211.1935	4211.1881	0.0054
0.270 (0 0 1 14 8)			
0.255 (0 0 1 14 10)			
	0.0000	4272.9989	0.0000
	0.0000	4337.7890	0.0000
0.265 (1 0 0 14 1)			
0.259 (1 0 0 14 11)			
	0.0000	4353.6266	0.0000
0.266 (0 0 1 14 4)			
0.311 (0 0 1 14 10)			
	0.0000	4364.3732	0.0000
0.318 (0 2 0 14 9)			
	0.0000	4426.4129	0.0000
0.251 (1 0 0 14 1)			
	0.0000	4460.3396	0.0000
	0.0000	4486.4080	0.0000
0.748 (0 2 0 14 13)			
	0.0000	4501.5314	0.0000
0.264 (1 0 0 14 9)			
	0.0000	4560.2887	0.0000
0.269 (0 0 1 14 10)			
0.338 (0 0 1 14 12)			
	4605.9795	4605.9779	0.0016
0.545 (1 0 0 14 13)			
	0.0000	4663.3160	0.0000
0.790 (0 0 1 14 14)			

SYMMETRY B1			
EIGENSTATE		Eexp	Ecalc
			Residual
		3547.2293	3547.2269
0.338	(0 2 0 14 2)		0.0024
0.464	(0 2 0 14 4)		
		3786.4795	3786.4780
0.327	(1 0 0 14 2)		0.0015
0.463	(1 0 0 14 4)		
		3803.4062	3803.4025
0.470	(0 0 1 14 3)		0.0037
0.331	(0 0 1 14 5)		
		3806.8735	3806.8771
0.315	(0 2 0 14 2)		-0.0036
0.369	(0 2 0 14 6)		
0.271	(0 2 0 14 8)		
		4011.8591	4011.8588
0.313	(1 0 0 14 2)		0.0003
0.352	(1 0 0 14 6)		
0.283	(1 0 0 14 8)		
		4016.4813	4016.4857
0.305	(0 2 0 14 8)		-0.0044
		4028.0103	4028.0067
0.409	(0 0 1 14 7)		0.0036
		0.0000	4178.4155
0.269	(0 2 0 14 4)		0.0000
0.340	(0 2 0 14 10)		
		4195.6728	4195.6759
0.282	(1 0 0 14 8)		-0.0031
		4211.1923	4211.1864
0.276	(0 0 1 14 5)		0.0059
0.377	(0 0 1 14 9)		
		0.0000	4303.3463
0.301	(0 2 0 14 8)		0.0000
0.282	(0 2 0 14 12)		
		4338.5905	4338.5924
0.268	(1 0 0 14 4)		-0.0019
0.325	(1 0 0 14 10)		
		0.0000	4353.2313
0.251	(0 0 1 14 1)		0.0000
0.279	(0 0 1 14 11)		
		0.0000	4424.3950
0.291	(0 2 0 14 10)		0.0000
0.504	(0 2 0 14 12)		
		4440.0039	4440.0001
		0.0000	4451.1773
		4512.1424	4512.1414
0.253	(0 0 1 14 9)		0.0010
		0.0000	4543.7342
0.891	(0 2 0 14 14)		0.0000
		4552.3483	4552.3370
0.260	(1 0 0 14 10)		0.0113
0.343	(1 0 0 14 12)		

	0.0000	4612.1234	0.0000
0.546 (0 0 1 14 13)	4659.2967	4659.2971	-0.0004
0.766 (1 0 0 14 14)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	3397.3235	3397.3229	0.0006
0.613 (0 2 0 14 1)			
0.304 (0 2 0 14 3)			
	3657.6057	3657.6084	-0.0027
0.604 (1 0 0 14 1)			
0.306 (1 0 0 14 3)			
	3675.0092	3675.0086	0.0006
0.327 (0 0 1 14 0)			
0.467 (0 0 1 14 2)			
	3683.5131	3683.5167	-0.0036
0.444 (0 2 0 14 5)			
	3904.4637	3904.4631	0.0006
0.434 (1 0 0 14 5)			
0.253 (1 0 0 14 7)			
	3917.7102	3917.7098	0.0004
0.314 (0 2 0 14 7)			
0.264 (0 2 0 14 9)			
	3921.0196	3921.0190	0.0006
0.264 (0 0 1 14 4)			
0.398 (0 0 1 14 6)			
	4103.2596	4103.2659	-0.0063
0.262 (0 2 0 14 3)			
0.321 (0 2 0 14 9)			
	4108.8879	4108.8922	-0.0043
0.297 (1 0 0 14 7)			
0.279 (1 0 0 14 9)			
	4124.6822	4124.6888	-0.0066
0.257 (0 0 1 14 4)			
0.395 (0 0 1 14 8)			
	0.0000	4243.6364	0.0000
0.256 (0 2 0 14 5)			
0.330 (0 2 0 14 11)			
	4272.2399	4272.2416	-0.0017
0.262 (1 0 0 14 3)			
0.300 (1 0 0 14 9)			
	4287.4974	4287.4948	0.0026
0.269 (0 0 1 14 6)			
0.346 (0 0 1 14 10)			
	0.0000	4362.8438	0.0000
0.328 (0 2 0 14 9)			
0.261 (0 2 0 14 11)			
	4395.1887	4395.1893	-0.0006
0.319 (1 0 0 14 11)			
	4406.8400	4406.8348	0.0052
	4472.7594	4472.7612	-0.0018

	0.0000	4486.3973	0.0000
0.748 (0 2 0 14 13)			
	4500.1290	4500.1272	0.0018
0.262 (1 0 0 14 9)			
	4560.5982	4560.5949	0.0033
0.268 (0 0 1 14 10)			
0.332 (0 0 1 14 12)			
	4605.9747	4605.9719	0.0028
0.545 (1 0 0 14 13)			
	0.0000	4663.3170	0.0000
0.789 (0 0 1 14 14)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	3701.3661	3701.3633	0.0028
0.315 (0 2 0 15 2)			
0.460 (0 2 0 15 4)			
	3939.5995	3939.5971	0.0024
0.303 (1 0 0 15 2)			
0.457 (1 0 0 15 4)			
	3956.9999	3956.9987	0.0012
0.451 (0 0 1 15 3)			
0.345 (0 0 1 15 5)			
	3982.0364	3982.0375	-0.0011
0.304 (0 2 0 15 2)			
0.323 (0 2 0 15 6)			
0.306 (0 2 0 15 8)			
	4183.2295	4183.2301	-0.0006
0.300 (1 0 0 15 2)			
0.303 (1 0 0 15 6)			
0.316 (1 0 0 15 8)			
	4199.7253	4199.7292	-0.0039
0.400 (0 0 1 15 7)			
	4211.9456	4211.9416	0.0040
0.288 (0 2 0 15 10)			
	4384.9057	4384.9031	0.0026
0.298 (1 0 0 15 10)			
	0.0000	4393.6135	0.0000
0.261 (0 2 0 15 4)			
0.275 (0 2 0 15 10)			
	0.0000	4400.7548	0.0000
0.269 (0 0 1 15 5)			
0.357 (0 0 1 15 9)			
	0.0000	4532.8106	0.0000
0.250 (0 2 0 15 6)			
0.318 (0 2 0 15 12)			
	0.0000	4545.6282	0.0000
0.255 (1 0 0 15 4)			
0.251 (1 0 0 15 10)			
	0.0000	4560.8494	0.0000
0.251 (0 0 1 15 7)			
0.323 (0 0 1 15 11)			

	0.0000	4658.3052	0.0000
0.325 (0 2 0 15 10)			
0.251 (0 2 0 15 12)			
	0.0000	4666.0489	0.0000
0.287 (1 0 0 15 12)			
	0.0000	4675.8193	0.0000
	0.0000	4742.0011	0.0000
	0.0000	4777.4105	0.0000
0.258 (1 0 0 15 10)			
	0.0000	4787.7819	0.0000
0.735 (0 2 0 15 14)			
	0.0000	4840.5395	0.0000
0.264 (0 0 1 15 11)			
0.311 (0 0 1 15 13)			
	0.0000	4889.2179	0.0000
0.508 (1 0 0 15 14)			
	0.0000	4947.1564	0.0000
0.756 (0 0 1 15 15)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	3540.3891	3540.3890	0.0001
0.597 (0 2 0 15 1)			
0.308 (0 2 0 15 3)			
	3801.3436	3801.3456	-0.0020
0.587 (1 0 0 15 1)			
0.310 (1 0 0 15 3)			
	3819.2408	3819.2427	-0.0019
0.317 (0 0 1 15 0)			
0.462 (0 0 1 15 2)			
	3848.3123	3848.3174	-0.0051
0.418 (0 2 0 15 5)			
0.270 (0 2 0 15 7)			
	4066.7782	4066.7780	0.0002
0.406 (1 0 0 15 5)			
0.280 (1 0 0 15 7)			
	4083.7122	4083.7124	-0.0002
0.407 (0 0 1 15 6)			
	4103.1155	4103.1111	0.0044
0.254 (0 2 0 15 7)			
0.309 (0 2 0 15 9)			
	4289.2128	4289.2141	-0.0013
0.319 (1 0 0 15 9)			
	0.0000	4305.2763	0.0000
0.258 (0 0 1 15 4)			
0.368 (0 0 1 15 8)			
	0.0000	4308.7956	0.0000
0.252 (0 2 0 15 3)			
	0.0000	4467.3837	0.0000
0.260 (0 2 0 15 5)			
0.310 (0 2 0 15 11)			
	4470.4068	4470.4071	-0.0003

0.254 (1 0 0 15 3)			
0.252 (1 0 0 15 11)			
	0.0000	4485.9372	0.0000
0.259 (0 0 1 15 6)			
0.348 (0 0 1 15 10)			
	0.0000	4594.9998	0.0000
0.294 (0 2 0 15 9)			
0.285 (0 2 0 15 13)			
	0.0000	4610.7307	0.0000
0.255 (1 0 0 15 5)			
0.291 (1 0 0 15 11)			
	0.0000	4624.6808	0.0000
0.259 (0 0 1 15 12)			
	0.0000	4706.2060	0.0000
	0.0000	4723.0113	0.0000
0.366 (0 2 0 15 13)			
	0.0000	4724.7423	0.0000
	0.0000	4787.7930	0.0000
0.255 (0 0 1 15 10)			
	0.0000	4833.0937	0.0000
0.256 (1 0 0 15 11)			
0.318 (1 0 0 15 13)			
	0.0000	4845.0687	0.0000
0.883 (0 2 0 15 15)			
	0.0000	4894.5167	0.0000
0.507 (0 0 1 15 14)			
	0.0000	4944.3049	0.0000
0.737 (1 0 0 15 15)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	3540.3891	3540.3890	0.0001
0.324 (0 2 0 15 0)			
0.466 (0 2 0 15 2)			
	3801.3436	3801.3456	-0.0020
0.318 (1 0 0 15 0)			
0.462 (1 0 0 15 2)			
	3819.2408	3819.2427	-0.0019
0.585 (0 0 1 15 1)			
0.311 (0 0 1 15 3)			
	3848.3123	3848.3174	-0.0051
0.252 (0 2 0 15 4)			
0.405 (0 2 0 15 6)			
	4066.7782	4066.7780	0.0002
0.406 (1 0 0 15 6)			
	4083.7122	4083.7124	-0.0002
0.401 (0 0 1 15 5)			
0.284 (0 0 1 15 7)			
	4103.1151	4103.1106	0.0045
0.259 (0 2 0 15 4)			
0.388 (0 2 0 15 8)			
	4289.2128	4289.2140	-0.0012

0.264 (1 0 0 15 4)			
0.379 (1 0 0 15 8)			
	0.0000	4305.2747	0.0000
0.318 (0 0 1 15 9)			
	0.0000	4308.7164	0.0000
0.259 (0 2 0 15 6)			
0.347 (0 2 0 15 10)			
	0.0000	4462.5893	0.0000
	4470.3670	4470.3682	-0.0012
0.263 (1 0 0 15 6)			
0.349 (1 0 0 15 10)			
	0.0000	4485.9420	0.0000
0.252 (0 0 1 15 3)			
0.263 (0 0 1 15 11)			
	0.0000	4553.6406	0.0000
	0.0000	4608.7143	0.0000
	0.0000	4625.7553	0.0000
0.250 (0 0 1 15 5)			
0.265 (0 0 1 15 11)			
	0.0000	4659.0851	0.0000
0.321 (0 2 0 15 10)			
	0.0000	4691.4519	0.0000
	0.0000	4734.0615	0.0000
	0.0000	4778.1121	0.0000
0.258 (1 0 0 15 10)			
	0.0000	4787.7913	0.0000
0.734 (0 2 0 15 14)			
	0.0000	4840.3874	0.0000
0.265 (0 0 1 15 11)			
0.313 (0 0 1 15 13)			
	0.0000	4889.2204	0.0000
0.508 (1 0 0 15 14)			
	0.0000	4947.1559	0.0000
0.756 (0 0 1 15 15)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	3701.3661	3701.3633	0.0028
0.466 (0 2 0 15 3)			
0.337 (0 2 0 15 5)			
	3939.5995	3939.5971	0.0024
0.454 (1 0 0 15 3)			
0.343 (1 0 0 15 5)			
	3956.9999	3956.9987	0.0012
0.299 (0 0 1 15 2)			
0.457 (0 0 1 15 4)			
	3982.0364	3982.0375	-0.0011
0.406 (0 2 0 15 7)			
	4183.2295	4183.2301	-0.0006
0.402 (1 0 0 15 7)			
	4199.7253	4199.7292	-0.0039
0.296 (0 0 1 15 2)			

0.294 (0 0 1 15 6)			
0.320 (0 0 1 15 8)			
	4211.9391	4211.9349	0.0042
0.273 (0 2 0 15 5)			
0.371 (0 2 0 15 9)			
	4384.9037	4384.9013	0.0024
0.272 (1 0 0 15 5)			
0.362 (1 0 0 15 9)			
	0.0000	4392.8785	0.0000
0.312 (0 2 0 15 11)			
	0.0000	4400.7515	0.0000
0.304 (0 0 1 15 10)			
	0.0000	4513.8500	0.0000
0.280 (0 2 0 15 1)			
	4545.3796	4545.3742	0.0054
0.252 (1 0 0 15 7)			
0.316 (1 0 0 15 11)			
	0.0000	4560.9546	0.0000
	0.0000	4600.1793	0.0000
0.255 (0 2 0 15 9)			
0.254 (0 2 0 15 13)			
	0.0000	4656.6196	0.0000
0.291 (1 0 0 15 1)			
	0.0000	4681.8855	0.0000
	0.0000	4723.4146	0.0000
0.290 (0 2 0 15 11)			
0.480 (0 2 0 15 13)			
	0.0000	4729.3062	0.0000
	0.0000	4786.4125	0.0000
0.268 (0 0 1 15 10)			
	0.0000	4833.1528	0.0000
0.256 (1 0 0 15 11)			
0.318 (1 0 0 15 13)			
	0.0000	4845.0692	0.0000
0.883 (0 2 0 15 15)			
	0.0000	4894.5052	0.0000
0.507 (0 0 1 15 14)			
	0.0000	4944.3048	0.0000
0.737 (1 0 0 15 15)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	3692.5131	3692.5137	-0.0006
0.315 (0 2 0 16 0)			
0.461 (0 2 0 16 2)			
	3954.2177	3954.2195	-0.0018
0.309 (1 0 0 16 0)			
0.457 (1 0 0 16 2)			
	0.0000	3972.6455	0.0000
0.571 (0 0 1 16 1)			
0.314 (0 0 1 16 3)			
	4022.1348	4022.1423	-0.0075

0.406 (0 2 0 16 6)	4238.1538	4238.1528	0.0010
0.405 (1 0 0 16 6)	0.0000	4255.5450	0.0000
0.372 (0 0 1 16 5)			
0.305 (0 0 1 16 7)	0.0000	4297.3141	0.0000
0.263 (0 2 0 16 4)			
0.363 (0 2 0 16 8)	4478.4604	4478.4606	-0.0002
0.265 (1 0 0 16 4)			
0.349 (1 0 0 16 8)	4494.9555	4494.9568	-0.0013
0.346 (0 0 1 16 9)	0.0000	4522.7493	0.0000
0.335 (0 2 0 16 10)	0.0000	4677.2256	0.0000
0.319 (1 0 0 16 10)	0.0000	4692.9876	0.0000
0.305 (0 0 1 16 11)	0.0000	4698.7432	0.0000
0.285 (0 2 0 16 12)	0.0000	4810.2714	0.0000
	0.0000	4834.4094	0.0000
0.285 (1 0 0 16 12)	0.0000	4850.4651	0.0000
	0.0000	4907.8960	0.0000
0.268 (0 2 0 16 10)			
0.274 (0 2 0 16 14)	0.0000	4937.9491	0.0000
	0.0000	4970.7988	0.0000
	0.0000	5018.4458	0.0000
	0.0000	5040.5972	0.0000
0.296 (0 2 0 16 12)			
0.472 (0 2 0 16 14)	0.0000	5081.0997	0.0000
0.259 (0 0 1 16 11)	0.0000	5131.5285	0.0000
0.253 (1 0 0 16 12)			
0.294 (1 0 0 16 14)	0.0000	5162.9783	0.0000
0.873 (0 2 0 16 16)	0.0000	5194.0927	0.0000
0.462 (0 0 1 16 15)	0.0000	5246.2165	0.0000
0.701 (1 0 0 16 16)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	3864.5662	3864.5623	0.0039
0.445 (0 2 0 16 3)			
0.347 (0 2 0 16 5)			

	4101.8270	4101.8234	0.0036
0.433 (1 0 0 16 3)			
0.352 (1 0 0 16 5)			
	0.0000	4119.7185	0.0000
0.279 (0 0 1 16 2)			
0.449 (0 0 1 16 4)			
	0.0000	4166.1632	0.0000
0.394 (0 2 0 16 7)			
	4363.5961	4363.5970	-0.0009
0.385 (1 0 0 16 7)			
	4380.5213	4380.5206	0.0007
0.284 (0 0 1 16 2)			
0.341 (0 0 1 16 8)			
	0.0000	4416.0824	0.0000
0.264 (0 2 0 16 5)			
0.343 (0 2 0 16 9)			
	4582.9631	4582.9632	-0.0001
0.258 (1 0 0 16 5)			
0.325 (1 0 0 16 9)			
	0.0000	4599.0801	0.0000
0.334 (0 0 1 16 10)			
	0.0000	4617.2789	0.0000
0.327 (0 2 0 16 11)			
	0.0000	4761.1766	0.0000
0.309 (1 0 0 16 11)			
	0.0000	4763.4703	0.0000
0.283 (0 2 0 16 1)			
	0.0000	4776.9154	0.0000
0.261 (0 0 1 16 12)			
	0.0000	4853.2173	0.0000
	0.0000	4894.4721	0.0000
0.280 (1 0 0 16 1)			
	0.0000	4914.1013	0.0000
	0.0000	4972.2946	0.0000
0.260 (0 2 0 16 11)			
	0.0000	4974.3578	0.0000
	0.0000	5025.4310	0.0000
	0.0000	5073.0503	0.0000
0.255 (1 0 0 16 11)			
	0.0000	5106.5412	0.0000
0.725 (0 2 0 16 15)			
	0.0000	5138.0879	0.0000
0.261 (0 0 1 16 12)			
0.286 (0 0 1 16 14)			
	0.0000	5189.5283	0.0000
0.464 (1 0 0 16 15)			
	0.0000	5247.9335	0.0000
0.714 (0 0 1 16 16)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
3864.5662	3864.5623	0.0039	

0.294 (0 2 0 16 2)			
0.454 (0 2 0 16 4)			
	4101.8270	4101.8234	0.0036
0.282 (1 0 0 16 2)			
0.450 (1 0 0 16 4)			
	0.0000	4119.7185	0.0000
0.430 (0 0 1 16 3)			
0.354 (0 0 1 16 5)			
	0.0000	4166.1632	0.0000
0.291 (0 2 0 16 2)			
0.278 (0 2 0 16 6)			
0.330 (0 2 0 16 8)			
	4363.5961	4363.5970	-0.0009
0.287 (1 0 0 16 2)			
0.255 (1 0 0 16 6)			
0.337 (1 0 0 16 8)			
	4380.5213	4380.5206	0.0007
0.382 (0 0 1 16 7)			
	0.0000	4416.0845	0.0000
0.325 (0 2 0 16 10)			
	4582.9634	4582.9637	-0.0003
0.330 (1 0 0 16 10)			
	0.0000	4599.0802	0.0000
0.253 (0 0 1 16 5)			
0.318 (0 0 1 16 9)			
	0.0000	4617.5355	0.0000
	0.0000	4761.2775	0.0000
0.252 (1 0 0 16 12)			
	0.0000	4773.2794	0.0000
0.279 (0 2 0 16 12)			
	0.0000	4776.9806	0.0000
0.303 (0 0 1 16 11)			
	0.0000	4898.8701	0.0000
0.260 (1 0 0 16 12)			
	0.0000	4905.2067	0.0000
0.284 (0 2 0 16 10)			
0.284 (0 2 0 16 14)			
	0.0000	4911.5390	0.0000
	0.0000	4988.6884	0.0000
	0.0000	5015.7164	0.0000
	0.0000	5040.5600	0.0000
0.296 (0 2 0 16 12)			
0.473 (0 2 0 16 14)			
	0.0000	5081.8089	0.0000
0.253 (0 0 1 16 11)			
	0.0000	5131.5015	0.0000
0.253 (1 0 0 16 12)			
0.294 (1 0 0 16 14)			
	0.0000	5162.9782	0.0000
0.873 (0 2 0 16 16)			
	0.0000	5194.0984	0.0000
0.461 (0 0 1 16 15)			

	0.0000	5246.2166	0.0000
0.701 (1 0 0 16 16)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	3692.5131	3692.5137	-0.0006
0.583 (0 2 0 16 1)			
0.312 (0 2 0 16 3)			
	3954.2177	3954.2195	-0.0018
0.573 (1 0 0 16 1)			
0.313 (1 0 0 16 3)			
	0.0000	3972.6455	0.0000
0.308 (0 0 1 16 0)			
0.456 (0 0 1 16 2)			
	4022.1348	4022.1423	-0.0075
0.392 (0 2 0 16 5)			
0.292 (0 2 0 16 7)			
	4238.1538	4238.1528	0.0010
0.377 (1 0 0 16 5)			
0.301 (1 0 0 16 7)			
	0.0000	4255.5450	0.0000
0.405 (0 0 1 16 6)			
	0.0000	4297.3143	0.0000
0.337 (0 2 0 16 9)			
	4478.4604	4478.4606	-0.0002
0.342 (1 0 0 16 9)			
	4494.9555	4494.9568	-0.0013
0.265 (0 0 1 16 4)			
0.343 (0 0 1 16 8)			
	0.0000	4522.7751	0.0000
0.295 (0 2 0 16 11)			
	0.0000	4677.2317	0.0000
0.302 (1 0 0 16 11)			
	0.0000	4693.0049	0.0000
0.310 (0 0 1 16 10)			
	0.0000	4700.6481	0.0000
	0.0000	4835.0413	0.0000
	0.0000	4839.8635	0.0000
0.307 (0 2 0 16 13)			
	0.0000	4850.1658	0.0000
0.296 (0 0 1 16 12)			
	0.0000	4951.1966	0.0000
	0.0000	4962.0060	0.0000
	0.0000	4972.4282	0.0000
0.322 (0 2 0 16 11)			
	0.0000	5030.0823	0.0000
	0.0000	5072.7082	0.0000
0.255 (1 0 0 16 11)			
	0.0000	5106.5386	0.0000
0.725 (0 2 0 16 15)			
	0.0000	5138.1629	0.0000
0.260 (0 0 1 16 12)			

0.284	(0 0 1 16 14)	0.0000	5189.5273	0.0000
0.463	(1 0 0 16 15)	0.0000	5247.9338	0.0000
0.714	(0 0 1 16 16)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
4036.8121	4036.8061	0.0060	
0.276 (0 2 0 17 2)			
0.447 (0 2 0 17 4)			
4273.1386	4273.1330	0.0056	
0.263 (1 0 0 17 2)			
0.441 (1 0 0 17 4)			
0.0000	4291.5527	0.0000	
0.410 (0 0 1 17 3)			
0.360 (0 0 1 17 5)			
0.0000	4359.2183	0.0000	
0.279 (0 2 0 17 2)			
0.346 (0 2 0 17 8)			
0.0000	4552.9341	0.0000	
0.274 (1 0 0 17 2)			
0.350 (1 0 0 17 8)			
0.0000	4570.3050	0.0000	
0.357 (0 0 1 17 7)			
0.0000	4628.9425	0.0000	
0.341 (0 2 0 17 10)			
4789.8214	4789.8193	0.0021	
0.339 (1 0 0 17 10)			
0.0000	4806.3036	0.0000	
0.266 (0 0 1 17 9)			
0.0000	4849.8631	0.0000	
0.293 (0 2 0 17 12)			
0.0000	4985.5183	0.0000	
0.294 (1 0 0 17 12)			
0.0000	5001.3419	0.0000	
0.264 (0 0 1 17 11)			
0.0000	5023.8833	0.0000	
0.0000	5140.3249	0.0000	
0.0000	5154.7394	0.0000	
0.268 (0 0 1 17 13)			
0.0000	5164.8361	0.0000	
0.309 (0 2 0 17 14)			
0.0000	5249.7676	0.0000	
0.0000	5266.9493	0.0000	
0.0000	5304.4148	0.0000	
0.322 (0 2 0 17 12)			
0.0000	5336.8936	0.0000	
0.0000	5385.5364	0.0000	
0.0000	5442.1839	0.0000	
0.709 (0 2 0 17 16)			
0.0000	5453.0976	0.0000	

0.255	(1 0 0 17 16)			
0.254	(0 0 1 17 13)			
0.254	(0 0 1 17 15)			
		0.0000	5506.4518	0.0000
0.413	(1 0 0 17 16)			
		0.0000	5565.4267	0.0000
0.662	(0 0 1 17 17)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	3853.6765	0.0000
0.570 (0 2 0 17 1)			
0.314 (0 2 0 17 3)			
	4116.2061	4116.2071	-0.0010
0.559 (1 0 0 17 1)			
0.315 (1 0 0 17 3)			
	0.0000	4135.1953	0.0000
0.299 (0 0 1 17 0)			
0.451 (0 0 1 17 2)			
	0.0000	4204.9714	0.0000
0.366 (0 2 0 17 5)			
0.310 (0 2 0 17 7)			
	4418.5633	4418.5620	0.0013
0.349 (1 0 0 17 5)			
0.317 (1 0 0 17 7)			
	0.0000	4436.4408	0.0000
0.399 (0 0 1 17 6)			
	0.0000	4500.3482	0.0000
0.351 (0 2 0 17 9)			
	4676.5977	4676.5986	-0.0009
0.351 (1 0 0 17 9)			
	0.0000	4693.5021	0.0000
0.260 (0 0 1 17 4)			
0.302 (0 0 1 17 8)			
0.254 (0 0 1 17 10)			
	0.0000	4745.3810	0.0000
0.324 (0 2 0 17 11)			
	0.0000	4892.7689	0.0000
0.322 (1 0 0 17 11)			
	0.0000	4908.8937	0.0000
0.255 (0 0 1 17 10)			
	0.0000	4942.5001	0.0000
	0.0000	5068.0252	0.0000
	0.0000	5083.5217	0.0000
0.277 (0 0 1 17 12)			
	0.0000	5096.4058	0.0000
0.276 (0 2 0 17 13)			
	0.0000	5202.6638	0.0000
	0.0000	5213.3050	0.0000
	0.0000	5233.7032	0.0000
0.285 (0 2 0 17 11)			
0.298 (0 2 0 17 15)			

	0.0000	5288.7175	0.0000
	0.0000	5324.9685	0.0000
	0.0000	5375.1220	0.0000
0.299 (0 2 0 17 13)			
0.453 (0 2 0 17 15)			
	0.0000	5393.7012	0.0000
	0.0000	5447.0753	0.0000
0.265 (1 0 0 17 15)			
	0.0000	5496.8431	0.0000
0.850 (0 2 0 17 17)			
	0.0000	5510.5658	0.0000
0.407 (0 0 1 17 16)			
	0.0000	5564.7805	0.0000
0.657 (1 0 0 17 17)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	3853.6765	0.0000
0.307 (0 2 0 17 0)			
0.456 (0 2 0 17 2)			
	4116.2061	4116.2071	-0.0010
0.300 (1 0 0 17 0)			
0.451 (1 0 0 17 2)			
	0.0000	4135.1953	0.0000
0.558 (0 0 1 17 1)			
0.316 (0 0 1 17 3)			
	0.0000	4204.9714	0.0000
0.403 (0 2 0 17 6)			
	4418.5633	4418.5620	0.0013
0.399 (1 0 0 17 6)			
	0.0000	4436.4408	0.0000
0.344 (0 0 1 17 5)			
0.321 (0 0 1 17 7)			
	0.0000	4500.3482	0.0000
0.262 (0 2 0 17 4)			
0.329 (0 2 0 17 8)			
	4676.5977	4676.5987	-0.0010
0.262 (1 0 0 17 4)			
0.309 (1 0 0 17 8)			
	0.0000	4693.5020	0.0000
0.352 (0 0 1 17 9)			
	0.0000	4745.3731	0.0000
0.290 (0 2 0 17 10)			
	0.0000	4892.7677	0.0000
0.265 (1 0 0 17 10)			
	0.0000	4908.8932	0.0000
0.325 (0 0 1 17 11)			
	0.0000	4941.7753	0.0000
0.298 (0 2 0 17 12)			
	0.0000	5067.7993	0.0000
0.280 (1 0 0 17 12)			
	0.0000	5078.1996	0.0000

	0.0000	5083.8107	0.0000
	0.0000	5172.5185	0.0000
0.262 (0 2 0 17 14)	0.0000	5194.2203	0.0000
	0.0000	5218.6958	0.0000
	0.0000	5274.7604	0.0000
	0.0000	5304.5846	0.0000
0.321 (0 2 0 17 12)	0.0000	5334.3466	0.0000
	0.0000	5385.6989	0.0000
	0.0000	5442.1850	0.0000
0.709 (0 2 0 17 16)	0.0000	5453.0607	0.0000
0.255 (1 0 0 17 16)			
0.254 (0 0 1 17 13)			
0.255 (0 0 1 17 15)			
	0.0000	5506.4522	0.0000
0.413 (1 0 0 17 16)			
	0.0000	5565.4265	0.0000
0.662 (0 0 1 17 17)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
	4036.8121	4036.8061	0.0060
0.426 (0 2 0 17 3)			
0.355 (0 2 0 17 5)			
	4273.1386	4273.1330	0.0056
0.413 (1 0 0 17 3)			
0.358 (1 0 0 17 5)			
	0.0000	4291.5527	0.0000
0.261 (0 0 1 17 2)			
0.441 (0 0 1 17 4)			
	0.0000	4359.2183	0.0000
0.375 (0 2 0 17 7)			
	0.0000	4552.9341	0.0000
0.361 (1 0 0 17 7)			
	0.0000	4570.3050	0.0000
0.272 (0 0 1 17 2)			
0.352 (0 0 1 17 8)			
	0.0000	4628.9416	0.0000
0.299 (0 2 0 17 9)			
	4789.8213	4789.8190	0.0023
0.275 (1 0 0 17 9)			
	0.0000	4806.3038	0.0000
0.341 (0 0 1 17 10)			
	0.0000	4849.7735	0.0000
0.297 (0 2 0 17 11)			
	0.0000	4985.4947	0.0000
0.273 (1 0 0 17 11)			
	0.0000	5001.3441	0.0000
0.299 (0 0 1 17 12)			
	0.0000	5019.3927	0.0000

0.262	(0 2 0 17 1)		
0.256	(0 2 0 17 13)		
		0.0000	5123.2324
		0.0000	5138.6150
		0.0000	5155.7516
		0.0000	5233.8837
		0.0000	5235.7008
		0.0000	5276.8002
		0.0000	5326.3910
		0.0000	5375.1380
0.299	(0 2 0 17 13)		
0.453	(0 2 0 17 15)		
		0.0000	5393.3452
		0.0000	5447.0875
0.265	(1 0 0 17 15)		
		0.0000	5496.8431
0.850	(0 2 0 17 17)		
		0.0000	5510.5629
0.407	(0 0 1 17 16)		
		0.0000	5564.7804
0.657	(1 0 0 17 17)		

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	4023.8521	4023.8553	-0.0032
0.299 (0 2 0 18 0)			
0.451 (0 2 0 18 2)			
	4287.2831	4287.2838	-0.0007
0.292 (1 0 0 18 0)			
0.445 (1 0 0 18 2)			
	0.0000	4306.8674	0.0000
0.546 (0 0 1 18 1)			
0.318 (0 0 1 18 3)			
	0.0000	4396.7843	0.0000
0.397 (0 2 0 18 6)			
	4607.9782	4607.9790	-0.0008
0.390 (1 0 0 18 6)			
	0.0000	4626.3732	0.0000
0.318 (0 0 1 18 5)			
0.332 (0 0 1 18 7)			
	0.0000	4712.1871	0.0000
0.257 (0 2 0 18 4)			
0.291 (0 2 0 18 8)			
0.266 (0 2 0 18 10)			
	0.0000	4883.5995	0.0000
0.254 (1 0 0 18 4)			
0.267 (1 0 0 18 8)			
0.276 (1 0 0 18 10)			
	0.0000	4900.9355	0.0000
0.346 (0 0 1 18 9)			
	0.0000	4976.5363	0.0000
	0.0000	5116.9656	0.0000

0.257 (1 0 0 18 12)	0.0000	5133.4309	0.0000
0.316 (0 0 1 18 11)	0.0000	5192.5366	0.0000
0.261 (0 2 0 18 12)	0.0000	5309.3323	0.0000
	0.0000	5325.2612	0.0000
0.282 (0 0 1 18 13)	0.0000	5353.9738	0.0000
	0.0000	5453.9957	0.0000
	0.0000	5457.2213	0.0000
	0.0000	5476.6259	0.0000
	0.0000	5547.6341	0.0000
	0.0000	5580.6458	0.0000
0.274 (0 2 0 18 12)			
0.301 (0 2 0 18 16)	0.0000	5599.8966	0.0000
	0.0000	5652.4001	0.0000
	0.0000	5722.8153	0.0000
	0.0000	5726.5289	0.0000
0.302 (0 2 0 18 14)			
0.431 (0 2 0 18 16)	0.0000	5779.4247	0.0000
0.284 (0 0 1 18 17)	0.0000	5841.9658	0.0000
0.263 (1 0 0 18 18)			
0.272 (0 0 1 18 17)	0.0000	5847.4685	0.0000
0.673 (0 2 0 18 18)	0.0000	5899.7906	0.0000
0.605 (1 0 0 18 18)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	4218.0752	0.0000	
0.408 (0 2 0 18 3)			
0.360 (0 2 0 18 5)	4453.5063	4453.5005	0.0058
0.394 (1 0 0 18 3)			
0.362 (1 0 0 18 5)	0.0000	4472.4754	0.0000
0.432 (0 0 1 18 4)	0.0000	4561.1798	0.0000
0.351 (0 2 0 18 7)	4751.2094	4751.2131	-0.0037
0.334 (1 0 0 18 7)			
0.257 (1 0 0 18 9)	0.0000	4769.0590	0.0000
0.260 (0 0 1 18 2)			
0.356 (0 0 1 18 8)	0.0000	4850.4856	0.0000
0.266 (0 2 0 18 11)			

	0.0000	5005.4441	0.0000
0.275 (1 0 0 18 11)	0.0000	5022.3175	0.0000
0.330 (0 0 1 18 10)	0.0000	5090.5767	0.0000
	0.0000	5218.2741	0.0000
	0.0000	5234.4126	0.0000
0.304 (0 0 1 18 12)	0.0000	5281.4493	0.0000
0.269 (0 2 0 18 13)	0.0000	5389.6381	0.0000
	0.0000	5405.3432	0.0000
	0.0000	5408.0389	0.0000
	0.0000	5507.3853	0.0000
	0.0000	5511.7984	0.0000
0.268 (0 2 0 18 15)	0.0000	5539.6796	0.0000
	0.0000	5594.3779	0.0000
	0.0000	5653.9153	0.0000
0.315 (0 2 0 18 13)	0.0000	5660.6916	0.0000
	0.0000	5715.6295	0.0000
	0.0000	5784.8521	0.0000
0.286 (1 0 0 18 17)	0.0000	5794.1043	0.0000
0.691 (0 2 0 18 17)	0.0000	5839.5553	0.0000
0.355 (1 0 0 18 17)			
0.305 (0 0 1 18 18)	0.0000	5899.4455	0.0000
0.600 (0 0 1 18 18)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	4218.0752	0.0000
0.259 (0 2 0 18 2)			
0.439 (0 2 0 18 4)			
	4453.5063	4453.5005	0.0058
0.432 (1 0 0 18 4)	0.0000	4472.4754	0.0000
0.392 (0 0 1 18 3)			
0.364 (0 0 1 18 5)	0.0000	4561.1798	0.0000
0.268 (0 2 0 18 2)			
0.354 (0 2 0 18 8)			
	4751.2094	4751.2131	-0.0037
0.262 (1 0 0 18 2)			
0.354 (1 0 0 18 8)	0.0000	4769.0590	0.0000
0.330 (0 0 1 18 7)			
0.262 (0 0 1 18 9)	0.0000	4850.4862	0.0000

0.340 (0 2 0 18 10)	0.0000	5005.4447	0.0000
0.331 (1 0 0 18 10)	0.0000	5022.3169	0.0000
0.281 (0 0 1 18 11)	0.0000	5090.6100	0.0000
0.312 (0 2 0 18 12)	0.0000	5218.2839	0.0000
0.304 (1 0 0 18 12)	0.0000	5234.4079	0.0000
	0.0000	5283.3174	0.0000
	0.0000	5390.2677	0.0000
	0.0000	5405.6090	0.0000
	0.0000	5436.3690	0.0000
0.268 (0 2 0 18 14)	0.0000	5520.4451	0.0000
	0.0000	5531.2389	0.0000
	0.0000	5580.0068	0.0000
0.280 (0 2 0 18 12)			
0.307 (0 2 0 18 16)	0.0000	5607.1082	0.0000
	0.0000	5651.6897	0.0000
	0.0000	5722.9910	0.0000
	0.0000	5726.5218	0.0000
0.302 (0 2 0 18 14)			
0.431 (0 2 0 18 16)	0.0000	5779.4191	0.0000
0.284 (0 0 1 18 17)	0.0000	5841.9670	0.0000
0.263 (1 0 0 18 18)			
0.272 (0 0 1 18 17)	0.0000	5847.4688	0.0000
0.673 (0 2 0 18 18)	0.0000	5899.7906	0.0000
0.605 (1 0 0 18 18)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
4023.8521	4023.8553	-0.0032	
0.558 (0 2 0 18 1)			
0.316 (0 2 0 18 3)	4287.2831	4287.2838	-0.0007
0.546 (1 0 0 18 1)			
0.316 (1 0 0 18 3)	0.0000	4306.8674	0.0000
0.292 (0 0 1 18 0)			
0.446 (0 0 1 18 2)	0.0000	4396.7843	0.0000
0.340 (0 2 0 18 5)			
0.323 (0 2 0 18 7)	4607.9782	4607.9790	-0.0008
0.322 (1 0 0 18 5)			

0.329 (1 0 0 18 7)	0.0000	4626.3732	0.0000
0.389 (0 0 1 18 6)	0.0000	4712.1870	0.0000
0.352 (0 2 0 18 9)	0.0000	4883.5993	0.0000
0.347 (1 0 0 18 9)	0.0000	4900.9356	0.0000
0.252 (0 0 1 18 4)			
0.259 (0 0 1 18 8)			
0.282 (0 0 1 18 10)	0.0000	4976.5379	0.0000
0.328 (0 2 0 18 11)	0.0000	5116.9647	0.0000
0.317 (1 0 0 18 11)	0.0000	5133.4323	0.0000
0.264 (0 0 1 18 12)	0.0000	5192.8004	0.0000
0.285 (0 2 0 18 13)	0.0000	5309.4007	0.0000
0.279 (1 0 0 18 13)	0.0000	5325.2454	0.0000
	0.0000	5363.3334	0.0000
	0.0000	5461.0398	0.0000
	0.0000	5474.2449	0.0000
	0.0000	5507.4749	0.0000
0.313 (0 2 0 18 15)	0.0000	5563.2458	0.0000
	0.0000	5589.8322	0.0000
	0.0000	5653.8515	0.0000
0.316 (0 2 0 18 13)	0.0000	5662.0089	0.0000
	0.0000	5715.5531	0.0000
	0.0000	5784.8703	0.0000
0.286 (1 0 0 18 17)	0.0000	5794.1037	0.0000
0.691 (0 2 0 18 17)	0.0000	5839.5552	0.0000
0.355 (1 0 0 18 17)			
0.305 (0 0 1 18 18)	0.0000	5899.4456	0.0000
0.600 (0 0 1 18 18)			

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	4408.3485	0.0000
0.431 (0 2 0 19 4)	4642.9049	4642.8996	0.0053
0.422 (1 0 0 19 4)			
0.253 (1 0 0 19 6)	0.0000	4662.4585	0.0000
0.375 (0 0 1 19 3)			

0.367 (0 0 1 19 5)	0.0000	4772.0228	0.0000
0.256 (0 2 0 19 2)			
0.356 (0 2 0 19 8)	0.0000	4958.4047	0.0000
0.251 (1 0 0 19 2)			
0.352 (1 0 0 19 8)	0.0000	4976.7512	0.0000
0.301 (0 0 1 19 7)			
0.281 (0 0 1 19 9)	0.0000	5080.6871	0.0000
0.325 (0 2 0 19 10)	0.0000	5229.8095	0.0000
0.309 (1 0 0 19 10)	0.0000	5247.0925	0.0000
0.300 (0 0 1 19 11)	0.0000	5339.7411	0.0000
0.304 (0 2 0 19 12)	0.0000	5459.5561	0.0000
0.285 (1 0 0 19 12)	0.0000	5475.9879	0.0000
0.268 (0 0 1 19 13)	0.0000	5551.2300	0.0000
0.273 (0 2 0 19 14)	0.0000	5648.5310	0.0000
0.259 (1 0 0 19 14)	0.0000	5664.3180	0.0000
	0.0000	5718.9809	0.0000
	0.0000	5796.7392	0.0000
	0.0000	5808.0334	0.0000
	0.0000	5867.6742	0.0000
0.315 (0 2 0 19 16)	0.0000	5893.3157	0.0000
	0.0000	5930.0706	0.0000
	0.0000	6004.6283	0.0000
	0.0000	6020.2495	0.0000
0.315 (0 2 0 19 14)			
0.256 (0 2 0 19 18)	0.0000	6062.3660	0.0000
	0.0000	6133.2689	0.0000
0.320 (1 0 0 19 18)	0.0000	6161.3250	0.0000
0.674 (0 2 0 19 18)	0.0000	6188.3685	0.0000
0.293 (1 0 0 19 18)			
0.370 (0 0 1 19 19)	0.0000	6249.8495	0.0000
0.529 (0 0 1 19 19)			

SYMMETRY A2

EIGENSTATE

0.0000	Eexp	Ecalc	Residual
	4203.0259		0.0000

0.546 (0 2 0 19 1)			
0.317 (0 2 0 19 3)			
	4467.4228	4467.4238	-0.0010
0.533 (1 0 0 19 1)			
0.317 (1 0 0 19 3)			
	0.0000	4487.6352	0.0000
0.285 (0 0 1 19 0)			
0.440 (0 0 1 19 2)			
	0.0000	4597.5591	0.0000
0.316 (0 2 0 19 5)			
0.332 (0 2 0 19 7)			
	4806.3710	4806.3760	-0.0050
0.296 (1 0 0 19 5)			
0.336 (1 0 0 19 7)			
	0.0000	4825.3125	0.0000
0.378 (0 0 1 19 6)			
	0.0000	4932.8023	0.0000
0.344 (0 2 0 19 9)			
	0.0000	5099.4321	0.0000
0.333 (1 0 0 19 9)			
	0.0000	5117.2258	0.0000
0.300 (0 0 1 19 10)			
	0.0000	5216.2198	0.0000
0.312 (0 2 0 19 11)			
	0.0000	5349.7927	0.0000
0.293 (1 0 0 19 11)			
	0.0000	5366.6235	0.0000
0.289 (0 0 1 19 12)			
	0.0000	5451.3826	0.0000
0.296 (0 2 0 19 13)			
	0.0000	5559.1444	0.0000
0.279 (1 0 0 19 13)			
	0.0000	5575.2690	0.0000
	0.0000	5639.7233	0.0000
	0.0000	5727.6706	0.0000
	0.0000	5742.4919	0.0000
	0.0000	5793.4213	0.0000
0.264 (0 2 0 19 15)			
	0.0000	5850.5828	0.0000
	0.0000	5867.0910	0.0000
	0.0000	5942.5250	0.0000
	0.0000	5945.1856	0.0000
	0.0000	5995.5547	0.0000
	0.0000	6069.2639	0.0000
	0.0000	6094.0176	0.0000
0.303 (0 2 0 19 15)			
0.408 (0 2 0 19 17)			
	0.0000	6128.1690	0.0000
0.321 (0 0 1 19 18)			
	0.0000	6191.2451	0.0000
0.358 (1 0 0 19 19)			
0.280 (0 0 1 19 18)			

	0.0000	6210.5693	0.0000
0.800 (0 2 0 19 19)	0.0000	6251.1160	0.0000
0.543 (1 0 0 19 19)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	4203.0259	0.0000	
0.292 (0 2 0 19 0)			
0.445 (0 2 0 19 2)			
4467.4228	4467.4238	-0.0010	
0.285 (1 0 0 19 0)			
0.439 (1 0 0 19 2)			
0.0000	4487.6352	0.0000	
0.535 (0 0 1 19 1)			
0.319 (0 0 1 19 3)			
0.0000	4597.5591	0.0000	
0.387 (0 2 0 19 6)			
4806.3710	4806.3760	-0.0050	
0.378 (1 0 0 19 6)			
0.0000	4825.3125	0.0000	
0.293 (0 0 1 19 5)			
0.339 (0 0 1 19 7)			
0.0000	4932.8026	0.0000	
0.251 (0 2 0 19 8)			
0.289 (0 2 0 19 10)			
0.0000	5099.4324	0.0000	
0.296 (1 0 0 19 10)			
0.0000	5117.2255	0.0000	
0.332 (0 0 1 19 9)			
0.0000	5216.2214	0.0000	
0.281 (0 2 0 19 12)			
0.0000	5349.7952	0.0000	
0.284 (1 0 0 19 12)			
0.0000	5366.6206	0.0000	
0.288 (0 0 1 19 11)			
0.0000	5451.2915	0.0000	
0.0000	5559.1273	0.0000	
0.0000	5575.2695	0.0000	
0.277 (0 0 1 19 13)			
0.0000	5635.4096	0.0000	
0.0000	5726.0879	0.0000	
0.0000	5743.1022	0.0000	
0.0000	5752.1460	0.0000	
0.0000	5835.1341	0.0000	
0.0000	5869.5488	0.0000	
0.285 (0 2 0 19 16)			
0.0000	5877.3553	0.0000	
0.0000	5932.5156	0.0000	
0.0000	6003.9558	0.0000	
0.0000	6020.2838	0.0000	
0.315 (0 2 0 19 14)			

0.256 (0 2 0 19 18)	0.0000	6062.4018	0.0000
	0.0000	6133.2598	0.0000
0.320 (1 0 0 19 18)	0.0000	6161.3253	0.0000
0.674 (0 2 0 19 18)	0.0000	6188.3685	0.0000
0.293 (1 0 0 19 18)			
0.370 (0 0 1 19 19)	0.0000	6249.8494	0.0000
0.529 (0 0 1 19 19)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	4408.3485	0.0000	
0.391 (0 2 0 19 3)			
0.363 (0 2 0 19 5)	4642.9049	4642.8996	0.0053
0.376 (1 0 0 19 3)			
0.364 (1 0 0 19 5)	0.0000	4662.4585	0.0000
0.423 (0 0 1 19 4)			
0.257 (0 0 1 19 6)	0.0000	4772.0227	0.0000
0.326 (0 2 0 19 7)			
0.267 (0 2 0 19 9)	0.0000	4958.4047	0.0000
0.305 (1 0 0 19 7)			
0.276 (1 0 0 19 9)	0.0000	4976.7513	0.0000
0.353 (0 0 1 19 8)	0.0000	5080.6860	0.0000
0.292 (0 2 0 19 11)	0.0000	5229.8084	0.0000
0.296 (1 0 0 19 11)	0.0000	5247.0936	0.0000
0.306 (0 0 1 19 10)	0.0000	5339.7254	0.0000
0.257 (0 2 0 19 13)	0.0000	5459.5488	0.0000
0.261 (1 0 0 19 13)	0.0000	5475.9937	0.0000
0.281 (0 0 1 19 12)	0.0000	5550.4838	0.0000
	0.0000	5648.3073	0.0000
	0.0000	5664.4054	0.0000
0.259 (0 0 1 19 14)	0.0000	5701.6596	0.0000
0.254 (0 2 0 19 1)	0.0000	5788.8887	0.0000
0.255 (1 0 0 19 1)	0.0000	5803.8705	0.0000

	0.0000	5813.2539	0.0000
	0.0000	5878.3210	0.0000
	0.0000	5939.4771	0.0000
	0.0000	5944.4853	0.0000
0.253	(0 2 0 19 13)		
0.295	(0 2 0 19 17)		
	0.0000	5995.9014	0.0000
	0.0000	6069.1774	0.0000
	0.0000	6094.0212	0.0000
0.303	(0 2 0 19 15)		
0.408	(0 2 0 19 17)		
	0.0000	6128.1716	0.0000
0.321	(0 0 1 19 18)		
	0.0000	6191.2443	0.0000
0.358	(1 0 0 19 19)		
0.280	(0 0 1 19 18)		
	0.0000	6210.5693	0.0000
0.800	(0 2 0 19 19)		
	0.0000	6251.1160	0.0000
0.543	(1 0 0 19 19)		

SYMMETRY A1

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	4391.1621	0.0000
0.286	(0 2 0 20 0)		
0.440	(0 2 0 20 2)		
	4656.5971	4656.5995	-0.0024
0.278	(1 0 0 20 0)		
0.433	(1 0 0 20 2)		
	0.0000	4677.4699	0.0000
0.524	(0 0 1 20 1)		
0.320	(0 0 1 20 3)		
	0.0000	4807.2718	0.0000
0.376	(0 2 0 20 6)		
	0.0000	5013.7244	0.0000
0.364	(1 0 0 20 6)		
	0.0000	5033.2266	0.0000
0.269	(0 0 1 20 5)		
0.343	(0 0 1 20 7)		
	0.0000	5162.1628	0.0000
0.304	(0 2 0 20 10)		
	0.0000	5324.0661	0.0000
0.307	(1 0 0 20 10)		
	0.0000	5342.3370	0.0000
0.311	(0 0 1 20 9)		
	0.0000	5464.3990	0.0000
0.299	(0 2 0 20 12)		
	0.0000	5591.2280	0.0000
0.295	(1 0 0 20 12)		
	0.0000	5608.4301	0.0000
	0.0000	5718.1625	0.0000
0.258	(0 2 0 20 14)		

	0.0000	5817.2335	0.0000
0.256 (1 0 0 20 14)	0.0000	5833.6187	0.0000
	0.0000	5922.9599	0.0000
	0.0000	6001.9527	0.0000
	0.0000	6018.3821	0.0000
	0.0000	6062.5032	0.0000
	0.0000	6133.5312	0.0000
	0.0000	6164.4404	0.0000
	0.0000	6174.0042	0.0000
	0.0000	6227.3377	0.0000
	0.0000	6296.6575	0.0000
	0.0000	6324.4858	0.0000
0.268 (0 2 0 20 14)			
0.325 (0 2 0 20 18)			
	0.0000	6356.3936	0.0000
	0.0000	6432.0614	0.0000
	0.0000	6476.7228	0.0000
0.302 (0 2 0 20 16)			
0.383 (0 2 0 20 18)			
	0.0000	6492.9138	0.0000
0.360 (0 0 1 20 19)			
	0.0000	6555.3619	0.0000
0.421 (1 0 0 20 20)			
	0.0000	6587.6335	0.0000
0.773 (0 2 0 20 20)			
	0.0000	6618.7142	0.0000
0.473 (1 0 0 20 20)			

SYMMETRY A2

EIGENSTATE	Eexp	Ecalc	Residual
	0.0000	4607.6031	0.0000
0.376 (0 2 0 20 3)			
0.364 (0 2 0 20 5)			
	4841.3026	4841.3026	0.0000
0.360 (1 0 0 20 3)			
0.365 (1 0 0 20 5)			
	0.0000	4861.4716	0.0000
0.413 (0 0 1 20 4)			
0.266 (0 0 1 20 6)			
	0.0000	4991.7191	0.0000
0.299 (0 2 0 20 7)			
0.283 (0 2 0 20 9)			
	0.0000	5174.4788	0.0000
0.276 (1 0 0 20 7)			
0.290 (1 0 0 20 9)			
	0.0000	5193.3481	0.0000
0.345 (0 0 1 20 8)			
	0.0000	5319.5091	0.0000
0.306 (0 2 0 20 11)			
	0.0000	5462.8802	0.0000
0.305 (1 0 0 20 11)			

	0.0000	5480.5970	0.0000
0.274 (0 0 1 20 10)	0.0000	5597.2175	0.0000
0.283 (0 2 0 20 13)	0.0000	5709.3031	0.0000
0.280 (1 0 0 20 13)	0.0000	5726.0708	0.0000
	0.0000	5827.0577	0.0000
	0.0000	5914.9328	0.0000
	0.0000	5931.1096	0.0000
	0.0000	6002.5676	0.0000
	0.0000	6076.2872	0.0000
	0.0000	6095.4459	0.0000
	0.0000	6113.4562	0.0000
	0.0000	6178.1370	0.0000
	0.0000	6230.5360	0.0000
	0.0000	6246.5357	0.0000
0.311 (0 2 0 20 17)	0.0000	6288.5965	0.0000
	0.0000	6364.1776	0.0000
	0.0000	6402.5997	0.0000
0.310 (0 2 0 20 15)			
0.270 (0 2 0 20 19)	0.0000	6425.6311	0.0000
0.251 (0 0 1 20 18)	0.0000	6497.8027	0.0000
0.356 (1 0 0 20 19)	0.0000	6542.8290	0.0000
0.638 (0 2 0 20 19)	0.0000	6552.5362	0.0000
0.432 (0 0 1 20 20)	0.0000	6616.5446	0.0000
0.451 (0 0 1 20 20)			

SYMMETRY B1

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	4607.6031	0.0000	
0.422 (0 2 0 20 4)			
0.255 (0 2 0 20 6)	4841.3026	4841.3026	0.0000
0.412 (1 0 0 20 4)			
0.262 (1 0 0 20 6)	0.0000	4861.4716	0.0000
0.360 (0 0 1 20 3)			
0.368 (0 0 1 20 5)	0.0000	4991.7193	0.0000
0.352 (0 2 0 20 8)	0.0000	5174.4789	0.0000
0.344 (1 0 0 20 8)	0.0000	5193.3479	0.0000
0.273 (0 0 1 20 7)			
0.295 (0 0 1 20 9)			

	0.0000	5319.5109	0.0000
0.301 (0 2 0 20 10)	0.0000	5462.8822	0.0000
0.278 (1 0 0 20 10)	0.0000	5480.5949	0.0000
0.308 (0 0 1 20 11)	0.0000	5597.2292	0.0000
0.275 (0 2 0 20 12)	0.0000	5709.3115	0.0000
	0.0000	5726.0627	0.0000
0.284 (0 0 1 20 13)	0.0000	5827.3529	0.0000
0.277 (0 2 0 20 14)	0.0000	5915.0151	0.0000
0.250 (1 0 0 20 14)	0.0000	5931.0757	0.0000
	0.0000	6011.5920	0.0000
	0.0000	6079.9420	0.0000
	0.0000	6093.5273	0.0000
	0.0000	6167.4187	0.0000
0.262 (0 2 0 20 16)	0.0000	6194.3409	0.0000
	0.0000	6220.5526	0.0000
	0.0000	6298.8025	0.0000
	0.0000	6324.3486	0.0000
0.268 (0 2 0 20 14)			
0.326 (0 2 0 20 18)	0.0000	6356.2257	0.0000
	0.0000	6432.1037	0.0000
	0.0000	6476.7210	0.0000
0.302 (0 2 0 20 16)			
0.383 (0 2 0 20 18)	0.0000	6492.9125	0.0000
0.360 (0 0 1 20 19)	0.0000	6555.3623	0.0000
0.421 (1 0 0 20 20)	0.0000	6587.6335	0.0000
0.773 (0 2 0 20 20)	0.0000	6618.7142	0.0000
0.473 (1 0 0 20 20)			

SYMMETRY B2

EIGENSTATE	Eexp	Ecalc	Residual
0.0000	4391.1621		0.0000
0.535 (0 2 0 20 1)			
0.317 (0 2 0 20 3)			
4656.5971	4656.5995		-0.0024
0.522 (1 0 0 20 1)			
0.317 (1 0 0 20 3)			
0.0000	4677.4699		0.0000
0.279 (0 0 1 20 0)			
0.435 (0 0 1 20 2)			

	0.0000	4807.2718	0.0000
0.293 (0 2 0 20 5)			
0.338 (0 2 0 20 7)			
	0.0000	5013.7244	0.0000
0.272 (1 0 0 20 5)			
0.340 (1 0 0 20 7)			
	0.0000	5033.2267	0.0000
0.365 (0 0 1 20 6)			
	0.0000	5162.1623	0.0000
0.329 (0 2 0 20 9)			
	0.0000	5324.0655	0.0000
0.313 (1 0 0 20 9)			
	0.0000	5342.3377	0.0000
0.311 (0 0 1 20 10)			
	0.0000	5464.3949	0.0000
0.281 (0 2 0 20 11)			
	0.0000	5591.2234	0.0000
0.255 (1 0 0 20 11)			
	0.0000	5608.4349	0.0000
0.298 (0 0 1 20 12)			
	0.0000	5718.1889	0.0000
0.277 (0 2 0 20 13)			
	0.0000	5817.2327	0.0000
	0.0000	5833.6251	0.0000
0.262 (0 0 1 20 14)			
	0.0000	5924.8098	0.0000
0.259 (0 2 0 20 15)			
	0.0000	6002.5507	0.0000
	0.0000	6018.1189	0.0000
	0.0000	6090.8562	0.0000
	0.0000	6146.0173	0.0000
	0.0000	6156.8589	0.0000
	0.0000	6240.1618	0.0000
	0.0000	6245.9845	0.0000
0.285 (0 2 0 20 17)			
	0.0000	6287.3384	0.0000
	0.0000	6364.5120	0.0000
	0.0000	6402.5831	0.0000
0.310 (0 2 0 20 15)			
0.270 (0 2 0 20 19)			
	0.0000	6425.6140	0.0000
0.251 (0 0 1 20 18)			
	0.0000	6497.8072	0.0000
0.355 (1 0 0 20 19)			
	0.0000	6542.8288	0.0000
0.638 (0 2 0 20 19)			
	0.0000	6552.5362	0.0000
0.432 (0 0 1 20 20)			
	0.0000	6616.5447	0.0000
0.451 (0 0 1 20 20)			