

Supporting Information for

Can a Single-Reference Approach Provide a Balanced Description of Ground and Excited States? A Comparison of the Completely Renormalized Equation-of-Motion Coupled-Cluster Method with Multi-Reference Quasi Degenerate Perturbation Theory Near a Conical Intersection and Along a Photodissociation Coordinate in Ammonia

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To be published in *J. Phys. Chem. A*

Date on which supporting information was prepared: October 25, 2005

S1. Adiabatic energies for scan 1 geometries.....	S-2
S2. Adiabatic energies for scan 2 geometries.....	S-3
S3. Adiabatic energies for scan 3 geometries.....	S-4
S4. Adiabatic energies for scan 4 geometries.....	S-5

Table S1. Adiabatic energies (hartrees) for the ground and first excited state of ammonia using CASSCF, MC-DQPT, CR-EOMCCSD(T), and EOMCCSD methods for scan 1 geometries obtained using the 6-311+G(3df,3pd) basis set.

R_A (Å)	CASSCF		MC-QDPT		CR-EOMCCSD(T)		EOMCCSD	
	V_1	V_2	V_1	V_2	V_1	V_2	V_1	V_2
0.80	-56.194	-56.007	-56.397	-56.183	-56.411	-56.186	-56.404	-56.183
0.90	-56.236	-56.054	-56.442	-56.232	-56.455	-56.236	-56.449	-56.233
1.00	-56.245	-56.067	-56.452	-56.249	-56.466	-56.253	-56.459	-56.249
1.10	-56.238	-56.064	-56.444	-56.251	-56.458	-56.253	-56.451	-56.249
1.20	-56.225	-56.056	-56.429	-56.249	-56.441	-56.247	-56.433	-56.243
1.30	-56.210	-56.054	-56.409	-56.237	-56.419	-56.244	-56.411	-56.238
1.40	-56.193	-56.061	-56.387	-56.236	-56.396	-56.245	-56.387	-56.237
1.50	-56.174	-56.069	-56.364	-56.242	-56.372	-56.249	-56.364	-56.239
1.60	-56.156	-56.078	-56.343	-56.244	-56.350	-56.254	-56.341	-56.242
1.80	-56.123	-56.093	-56.306	-56.261	-56.312	-56.264	-56.302	-56.247
1.90	-56.110	-56.099	-56.291	-56.273	-56.296	-56.268	-56.286	-56.248
2.00	-56.104	-56.099	-56.278	-56.273	-56.283	-56.271	-56.271	-56.250
2.10	-56.107	-56.090	-56.275	-56.268	-56.274	-56.272	-56.259	-56.250
2.20	-56.110	-56.083	-56.277	-56.259	-56.276	-56.262	-56.251	-56.248
2.30	-56.113	-56.077	-56.278	-56.252	-56.278	-56.255	-56.251	-56.240
2.40	-56.114	-56.073	-56.279	-56.247	-56.280	-56.249	-56.251	-56.233
2.60	-56.117	-56.067	-56.280	-56.239	-56.282	-56.240	-56.250	-56.222
2.80	-56.118	-56.063	-56.281	-56.235	-56.284	-56.235	-56.250	-56.215
3.00	-56.119	-56.061	-56.282	-56.232	-56.285	-56.233	-56.250	-56.211
5.00	-56.120	-56.059	-56.282	-56.229	-56.288	-56.230	-56.247	-56.202
7.00	-56.120	-56.059	-56.282	-56.229	-56.289	-56.230	-56.247	-56.202
9.00	-56.120	-56.059	-56.282	-56.229	-56.289	-56.230	-56.247	-56.202
11.00	-56.120	-56.059	-56.282	-56.229	-56.289	-56.230	-56.247	-56.202

Table S2. Adiabatic energies (hartrees) for the ground and first excited state of ammonia using CASSCF, MC-DQPT, CR-EOMCCSD(T), and EOMCCSD methods for scan 2 geometries obtained using the 6-311+G(3df,3pd) basis set.

R_A (Å)	CASSCF		MC-QDPT		CR-EOMCCSD(T)		EOMCCSD	
	V_1	V_2	V_1	V_2	V_1	V_2	V_1	V_2
0.80	-56.194	-56.007	-56.398	-56.182	-56.411	-56.186	-56.404	-56.183
0.90	-56.237	-56.054	-56.442	-56.232	-56.456	-56.235	-56.449	-56.233
1.00	-56.246	-56.067	-56.453	-56.248	-56.466	-56.252	-56.459	-56.249
1.10	-56.238	-56.064	-56.444	-56.250	-56.459	-56.252	-56.451	-56.249
1.20	-56.225	-56.056	-56.429	-56.248	-56.441	-56.247	-56.434	-56.243
1.30	-56.211	-56.054	-56.410	-56.237	-56.420	-56.243	-56.412	-56.237
1.40	-56.194	-56.060	-56.387	-56.235	-56.396	-56.244	-56.388	-56.236
1.50	-56.175	-56.068	-56.365	-56.241	-56.373	-56.248	-56.365	-56.238
1.60	-56.157	-56.077	-56.344	-56.242	-56.351	-56.253	-56.342	-56.241
1.90	-56.115	-56.094	-56.296	-56.266	-56.298	-56.265	-56.287	-56.246
2.00	-56.110	-56.093	-56.287	-56.265	-56.286	-56.267	-56.274	-56.246
2.10	-56.110	-56.088	-56.280	-56.263	-56.278	-56.265	-56.264	-56.244
2.20	-56.112	-56.082	-56.279	-56.257	-56.276	-56.257	-56.258	-56.238
2.30	-56.114	-56.076	-56.279	-56.251	-56.277	-56.247	-56.255	-56.230
2.60	-56.117	-56.066	-56.281	-56.239	-56.281	-56.237	-56.254	-56.211
2.80	-56.119	-56.063	-56.281	-56.235	-56.282	-56.236	-56.255	-56.205
3.00	-56.119	-56.061	-56.282	-56.232	-56.283	-56.236	-56.256	-56.201
5.00	-56.120	-56.059	-56.282	-56.229	-56.284	-56.238	-56.256	-56.195
7.00	-56.120	-56.059	-56.282	-56.229	-56.284	-56.238	-56.255	-56.195
9.00	-56.120	-56.059	-56.282	-56.229	-56.284	-56.238	-56.255	-56.194
11.00	-56.120	-56.059	-56.282	-56.229	-56.284	-56.238	-56.255	-56.194

Table S3. Adiabatic energies (hartrees) for the ground and first excited state of ammonia using CASSCF, MC-DQPT, CR-EOMCCSD(T), and EOMCCSD methods for scan 3 geometries obtained using the 6-311+G(3df,3pd) basis set.

R_A (Å)	CASSCF		MC-QDPT		CR-EOMCCSD(T)		EOMCCSD	
	V_1	V_2	V_1	V_2	V_1	V_2	V_1	V_2
0.80	-56.185	-56.000	-56.390	-56.177	-56.406	-56.181	-56.399	-56.178
0.90	-56.229	-56.047	-56.435	-56.226	-56.450	-56.230	-56.443	-56.227
1.00	-56.238	-56.061	-56.446	-56.243	-56.460	-56.247	-56.453	-56.244
1.10	-56.232	-56.058	-56.439	-56.244	-56.451	-56.248	-56.444	-56.244
1.20	-56.220	-56.051	-56.424	-56.244	-56.433	-56.244	-56.425	-56.239
1.30	-56.206	-56.050	-56.405	-56.237	-56.410	-56.243	-56.402	-56.236
1.40	-56.189	-56.055	-56.384	-56.233	-56.386	-56.246	-56.378	-56.238
1.50	-56.172	-56.064	-56.362	-56.238	-56.362	-56.252	-56.353	-56.241
1.60	-56.154	-56.072	-56.342	-56.241	-56.339	-56.258	-56.330	-56.245
1.80	-56.124	-56.087	-56.307	-56.260	-56.299	-56.268	-56.289	-56.252
1.90	-56.112	-56.092	-56.292	-56.267	-56.283	-56.273	-56.272	-56.254
2.00	-56.101	-56.097	-56.280	-56.267	-56.276	-56.268	-56.257	-56.255
2.10	-56.100	-56.093	-56.270	-56.269	-56.279	-56.256	-56.256	-56.244
2.20	-56.103	-56.086	-56.270	-56.262	-56.282	-56.247	-56.257	-56.233
2.30	-56.106	-56.081	-56.271	-56.256	-56.284	-56.238	-56.257	-56.224
2.40	-56.107	-56.076	-56.272	-56.251	-56.285	-56.232	-56.257	-56.216
2.60	-56.110	-56.071	-56.274	-56.244	-56.288	-56.223	-56.257	-56.205
2.80	-56.111	-56.067	-56.274	-56.239	-56.289	-56.218	-56.256	-56.198
3.00	-56.112	-56.066	-56.275	-56.237	-56.290	-56.215	-56.255	-56.193
5.00	-56.113	-56.064	-56.275	-56.234	-56.293	-56.212	-56.253	-56.185
7.00	-56.113	-56.064	-56.275	-56.234	-56.294	-56.212	-56.253	-56.184
9.00	-56.113	-56.064	-56.275	-56.234	-56.294	-56.212	-56.253	-56.184
11.00	-56.113	-56.064	-56.275	-56.234	-56.294	-56.213	-56.253	-56.184

Table S4. Adiabatic energies (hartrees) for the ground and first excited state of ammonia using CASSCF, MC-DQPT, CR-EOMCCSD(T), and EOMCCSD methods for scan 4 geometries obtained using the 6-311+G(3df,3pd) basis set.

R_A (Å)	CASSCF		MC-QDPT		CR-EOMCCSD(T)		EOMCCSD	
	V_1	V_2	V_1	V_2	V_1	V_2	V_1	V_2
0.80	-56.186	-55.999	-56.390	-56.176	-56.406	-56.180	-56.400	-56.178
0.90	-56.229	-56.047	-56.435	-56.226	-56.450	-56.230	-56.443	-56.227
1.00	-56.239	-56.061	-56.446	-56.243	-56.460	-56.247	-56.453	-56.244
1.10	-56.232	-56.058	-56.439	-56.243	-56.452	-56.247	-56.444	-56.244
1.20	-56.220	-56.051	-56.425	-56.246	-56.434	-56.243	-56.426	-56.239
1.30	-56.207	-56.049	-56.406	-56.237	-56.411	-56.242	-56.403	-56.236
1.40	-56.190	-56.054	-56.384	-56.233	-56.387	-56.245	-56.379	-56.237
1.50	-56.173	-56.063	-56.363	-56.237	-56.363	-56.251	-56.354	-56.240
1.60	-56.156	-56.071	-56.343	-56.240	-56.340	-56.256	-56.331	-56.244
1.80	-56.126	-56.085	-56.308	-56.252	-56.302	-56.266	-56.291	-56.249
1.90	-56.115	-56.089	-56.295	-56.263	-56.287	-56.267	-56.276	-56.248
2.00	-56.107	-56.091	-56.286	-56.262	-56.279	-56.261	-56.265	-56.243
2.10	-56.105	-56.089	-56.278	-56.261	-56.279	-56.248	-56.260	-56.232
2.20	-56.105	-56.084	-56.274	-56.259	-56.281	-56.238	-56.259	-56.220
2.30	-56.107	-56.079	-56.273	-56.254	-56.283	-56.232	-56.259	-56.211
2.40	-56.108	-56.076	-56.273	-56.250	-56.285	-56.228	-56.259	-56.203
2.60	-56.110	-56.070	-56.274	-56.243	-56.287	-56.223	-56.260	-56.192
2.80	-56.112	-56.067	-56.275	-56.239	-56.288	-56.221	-56.261	-56.186
3.00	-56.112	-56.065	-56.275	-56.237	-56.288	-56.220	-56.262	-56.182
5.00	-56.113	-56.064	-56.276	-56.234	-56.290	-56.220	-56.262	-56.177
7.00	-56.113	-56.064	-56.276	-56.234	-56.290	-56.220	-56.262	-56.177
9.00	-56.113	-56.064	-56.276	-56.234	-56.290	-56.220	-56.261	-56.176
11.00	-56.113	-56.064	-56.276	-56.234	-56.290	-56.220	-56.261	-56.176