Supporting Information

The Role of Vibronic Coupling in Maleimide: A Multi-Mode and Multi-State Quantum Dynamics Study

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Here we provide additional extensive information on the model Hamiltonian described in the manuscript and used for simulating absorption spectra and population transfer dynamics.

The number of electronic states to be considered is justified by calculating higher-lying singlet and triplet excited states as shown in Tab. S1. The EOM-CCSD/cc-pVDZ level of theory is compared to the EOM-CCSD/aug-cc-pVTZ level of theory, which has been employed along with the SA(11)-CASPT2(12,9)/cc-pVDZ to demonstate its applicability in the presented model Hamiltonian. ADC(3)/cc-pVDZ calculations, as another *ab initio* approach, are also listed for comparison. Fig. S1 shows the adiabatic potential energy surfaces along the normal modes ν_1 and ν_{18}. It is stressed that the inclusion of triplet states becomes crucial when simulating emission spectra. Singlet excited states above 7 eV are found to be energetically well separated from the first two excitation bands studied and seem to be based on complicated coupling between many excited states close in energy.
Fig. S2 shows all 24 normal modes together with their symmetries and the short-hand notation for the most dominant vibrations based on calculations at the CCSD/aug-cc-pVTZ level of theory being consistent with CCSD/cc-pVDZ results. Fig. S3 gives an overview of the adiabatic potential energy surfaces of all normal modes for the first five electronic states at the EOM-CCSD/cc-pVDZ level of theory which have been fitted in order to derive the model Hamiltonian.
A full list of on-diagonal linear intra-state coupling constants $\kappa_\alpha^{(i)}$, off-diagonal linear inter-state coupling constants $\lambda_\alpha^{(i,j)}$ as well as on-diagonal bilinear (quadratic) coupling constants $\gamma_{\alpha,\beta}^{(i)}$ ($\gamma_{\alpha,\alpha}^{(i)}$) can be found in Tab. S2, S3 and S4. Parameters concerning the diabatic quartic and Morse potential are displayed in Tab. S5 and S6. Furthermore, all parameters derived from this fitting procedure can also be seen from the MCTDH operator file showing the full structure of the Hamiltonian. The input file is given as well specifying the MCTDH parameters for the simulation of the second excitation band using the 6-mode model. Details on how to read this file can be found in the Quantics documentation.[1,2]
Based on this 6-mode model containing the most important normal modes of a_1 symmetry, the suggested peak assignment for the experimental second excitation band is shown in Fig. S4.

Table S1. Experimental and *ab initio* vertical singlet and triplet excitation energies E and oscillator strength f for maleimide in C_{2v} symmetry. While the EOM-CCSD/cc-pVDZ level of theory is chosen for calculating the points on the adiabatic PESs in Fig. S1, the EOM-CCSD/aug-cc-pVTZ, ADC(3)/cc-pVDZ and SA(11)-CASPT2(12,9)/cc-pVDZ results are shown here for comparison. The first five electronic states, $S_0 - S_4$ shown in bold letters, are considered in the presented model Hamiltonian.

		EOM-CCSD/ cc-pVDZ		**EOM-CCSD**/ aug-cc-pVTZ		**ADC(3)**/ cc-pVDZ		**SA(11)-CASPT2(12,9)**/ cc-pVDZ		**Experiment**	
state	sym	E / eV	f	E / eV	f	E / eV	f	E / eV	f	E / eV	
S_0	$1\,^1A_1$	0.00		0.00		0.00		0.00			
S_1	$1\,^1B_1$	4.06	0.000	4.14	0.000	3.81	0.000	3.37	0.001		3.33 [b]
S_2	$1\,^1A_2$	4.84	–	4.90	–	4.44	–	3.96	–		
S_3	$1\,^1B_2$	5.22	0.093	5.23	0.027	4.70	0.045	4.62	0.026	4.72 [a]	4.48 [b] 4.67 [c]
S_4	$2\,^1B_2$	6.68	0.432	6.55	0.450	6.11	0.503	5.80	0.456	∼5.95 [a]	∼6.20 [b,c]
S_5	$1\,^1B_1$	8.11	0.002	8.12	0.003	6.39	0.004				
S_6	$2\,^1A_2$	8.14	–	8.15	–	6.92	–	6.96	–		
S_7	$2\,^1A_1$	8.85	0.034	8.93	0.038	7.24	0.029	7.31	0.016		
S_8	$3\,^1B_1$	8.89	0.006	8.84	0.001	7.28	0.000	7.32	0.000		
S_9	$4\,^1B_1$	9.04	0.001	8.89	0.000	7.79	0.001	8.07	0.000		
S_{10}	$3\,^1B_2$	9.23	0.012	8.96	0.019	7.71	0.028				
T_1	$1\,^3B_2$	3.70	–	3.77	–	3.32	–				
T_2	$1\,^3B_1$	3.75	–	3.84	–	3.61	–				
T_3	$2\,^3B_2$	4.35	–	4.45	–	3.83	–				
T_4	$1\,^3A_2$	4.51	–	4.60	–	4.32	–				
T_5	$1\,^3A_1$	6.47	–	6.54	–	5.97	–				

[a] our vapour phase results at 315 K

[b] Seliskar *et al.*: maleimide in EPA mixed solvent at 77 K [3]

[c] Seliskar *et al.*: maleimide in 3-methylpentane at 300 K [3]

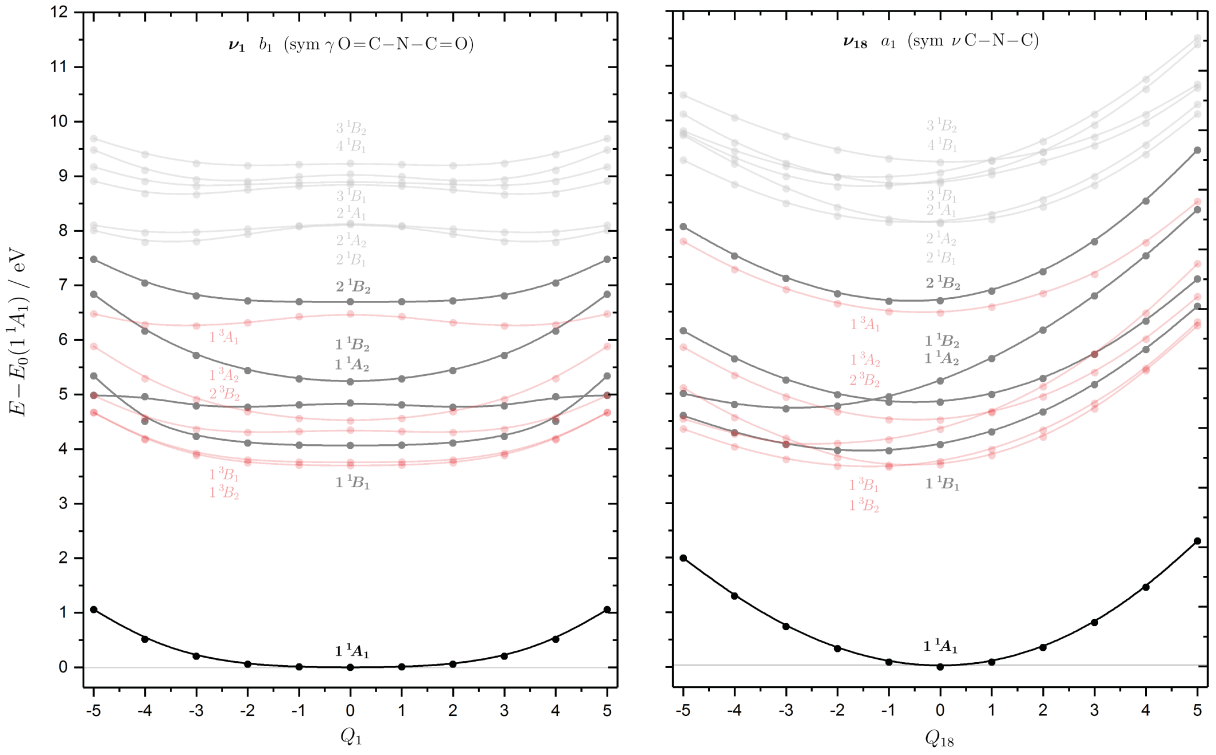

Figure S1. Adiabatic single-point energies E for a larger set of excited singlet and triplet states shown relative to the ground state energy at the FC point $E_0(^1A_1)$ as a function of mass- and frequency-scaled normal mode coordinates Q of mode ν_1 (left) and ν_{18} (right). The EOM-CCSD/cc-pVDZ level of theory has been chosen for calculating a wider range of excited states. The symmetry labels refer to the FC point at C_{2v} symmetry. The dark grey states of symmetry $1\,^1A_1$, $1\,^1B_1$, $1\,^1A_2$, $1\,^1B_2$ and $2\,^1B_2$ are treated explicitly, whereas states higher in energy (light grey) and triplet states (light red) are excluded in the presented model Hamiltonian.

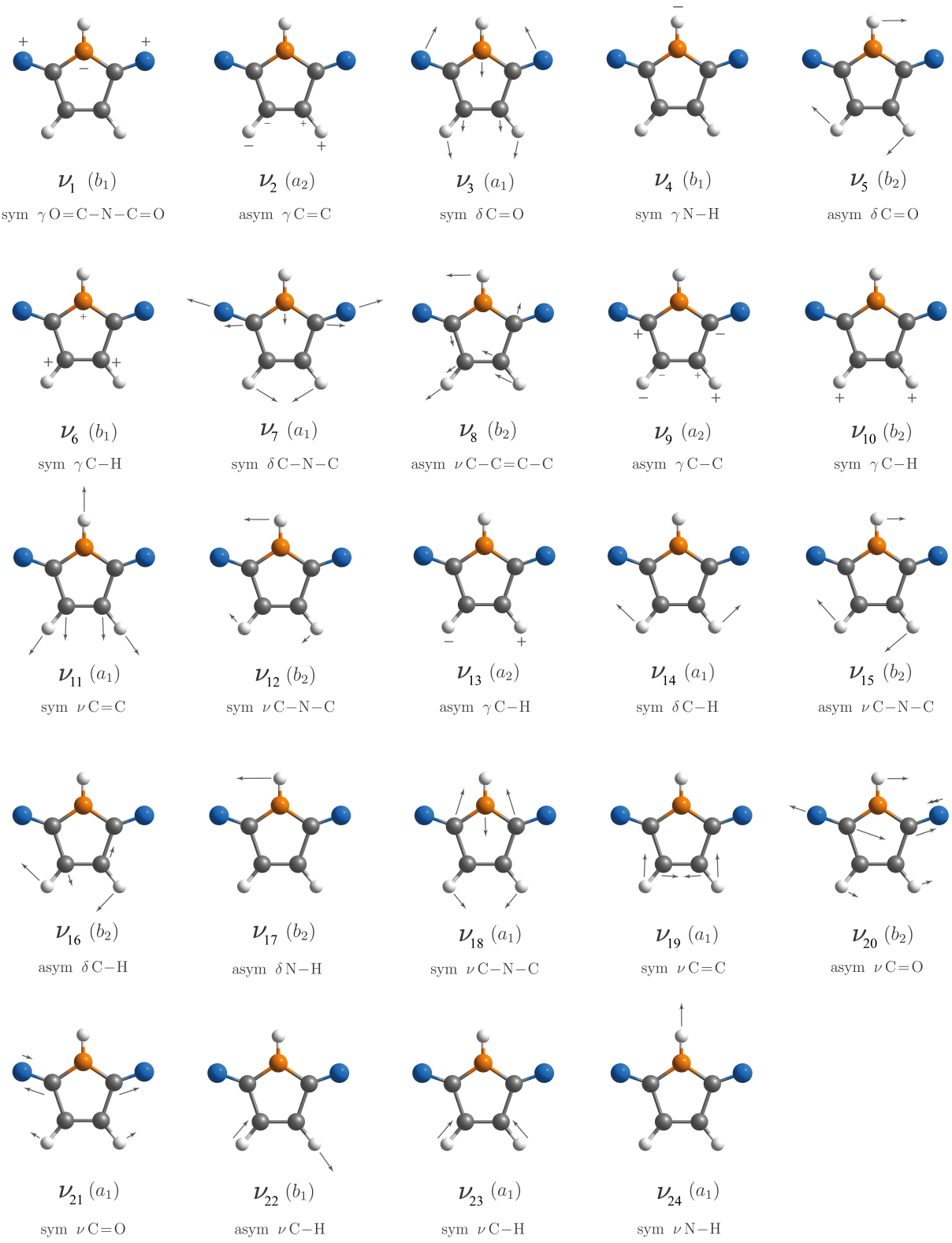

Figure S2. Overview of all normal modes ν, together with their point group symmetries and description of the most dominant molecular group partaking in the corresponding vibration. The results are based on CCSD/aug-cc-pVTZ frequency analyses. It is distinguished between streching (ν), bending (δ) and out-of-plane vibrations (γ). The labels *sym* and *asym* define the retained and broken symmetry with respect to the σ_v mirror plane perpendicular to the molecular plane.

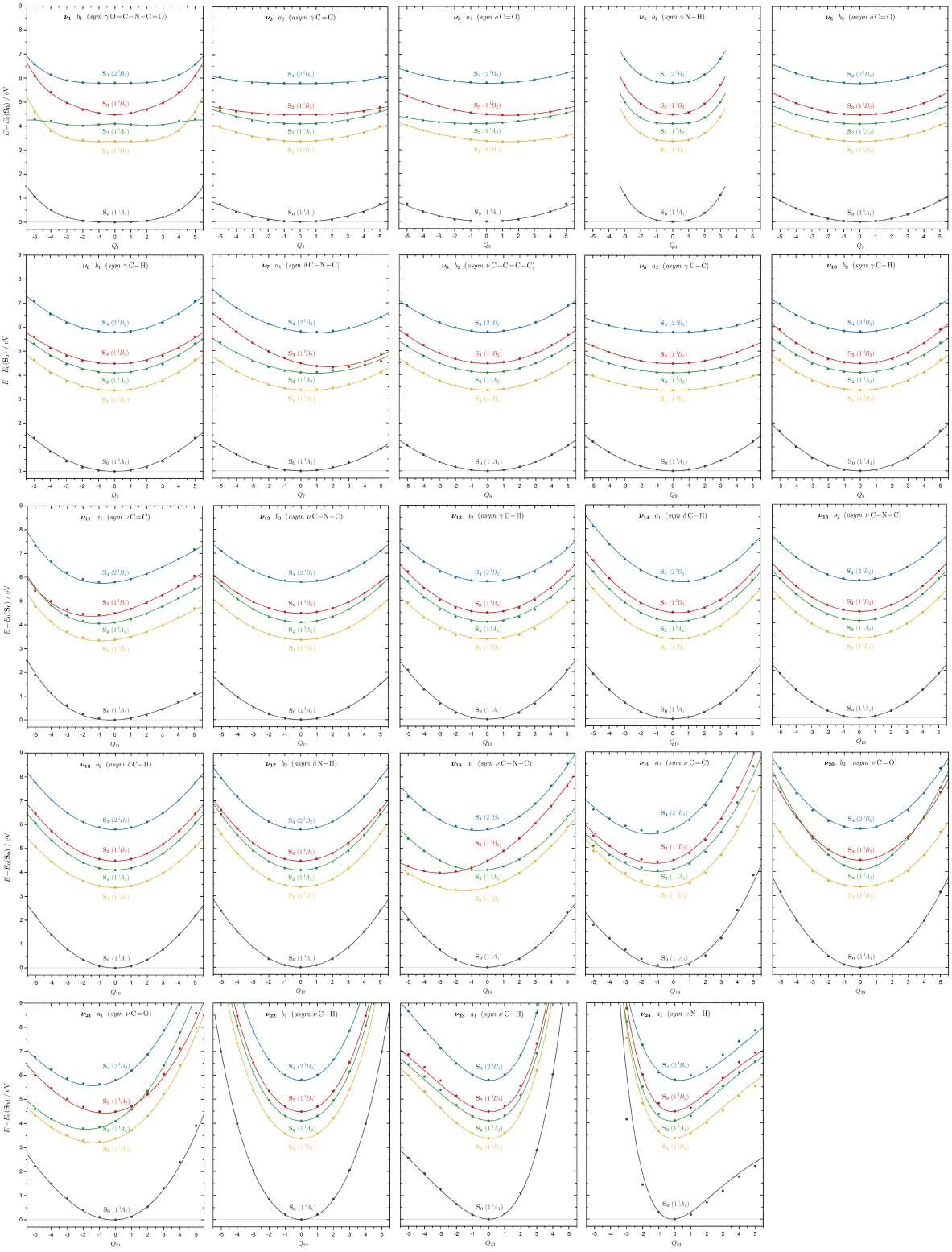

Figure S3. Adiabatic single-point energies E (dots) of maleimide calculated at the EOM-CCSD/cc-pVDZ level of theory for first five electronic states shown relative to the ground state energy at the FC point $E_0(S_0)$ as a function of mass- and frequency-scaled normal mode coordinates Q of all normal modes ν. The adiabatic potential energy curves (solid lines) are obtained from the fitted vibronic coupling model for that particular normal mode. Both the single-point energies as well as the fitted curves have been shifted to the SA(11)-CASPT2(12,9)/cc-pVDZ excitation energies. The ground state S_0 is shown in black, S_1 in yellow, S_2 in green, S_3 in red and S_4 in blue with symmetry labels referring to maleimide in C_{2v} symmetry at the FC point.

Table S2. On-diagonal linear intra-state coupling constants $\kappa_\alpha^{(i)}$ determined by fitting the adiabatic PESs for all vibrational modes. Corresponding frequencies ω and single-point energies have been calculated at the (EOM-)CCSD/cc-pVDZ level of theory. The parameter highlighted in red has been altered to achieve a better correspondence with the experiment (cf. Tab. 5).

mode	ω / eV	$\kappa_\alpha^{(i)}$ / eV			
		(1)	(2)	(3)	(4)
ν_3	0.049	-0.044	0.020	-0.054	-0.006
ν_7	0.080	-0.041	-0.065	-0.158	-0.078
ν_{11}	0.114	0.069	0.089	0.127	0.064
ν_{14}	0.133	-0.038	-0.037	-0.050	-0.086
ν_{18}	0.172	0.187	0.083	0.352	0.109
ν_{19}	0.206	0.049	0.130	0.169	0.229
ν_{21}	0.237	0.229	0.359	0.100	0.279
ν_{23}	0.408	-0.012	-0.014	-0.013	-0.027
ν_{24}	0.458	-0.006	0.007	-0.044	-0.010

Table S3. Off-diagonal linear inter-state coupling constants $\lambda_\alpha^{(i,j)}$ determined by fitting the adiabatic PESs for all vibrational modes. Corresponding frequencies ω and single-point energies have been calculated at the (EOM-)CCSD/cc-pVDZ level of theory. The parameter highlighted in red has been altered to achieve a better correspondence with the experiment (cf. Tab. 5).

mode	ω / eV	$\lambda_\alpha^{(i,j)}$ / eV									
		(0,1)	(0,2)	(0,3)	(0,4)	(1,2)	(1,3)	(1,4)	(2,3)	(2,4)	(3,4)
ν_1	0.014	-0.011							-0.131	-0.001	
ν_2	0.036		-0.011				0.055	-0.121			
ν_3	0.049										-0.061
ν_4	0.062	0.039							0.090	-0.076	
ν_5	0.067			0.001	-0.005	0.023					
ν_6	0.079	-0.023							0.005	0.035	
ν_7	0.080										-0.089
ν_8	0.084			-0.011	0.017	0.028					
ν_9	0.097		0.012				0.110	0.138			
ν_{10}	0.105	-0.037							-0.010	-0.075	
ν_{11}	0.114										0.048
ν_{12}	0.115			-0.009	0.012	0.005					
ν_{13}	0.119		-0.034				0.040	0.164			
ν_{14}	0.133										-0.002
ν_{15}	0.145			0.013	0.003	0.042					
ν_{16}	0.167			-0.019	-0.006	-0.036					
ν_{17}	0.170			0.008	0.001	0.035					
ν_{18}	0.172										0.071
ν_{19}	0.206										-0.028
ν_{20}	0.232			0.047	-0.109	-0.172					
ν_{21}	0.237										-0.029
ν_{22}	0.405			-0.002	0.001	-0.013					
ν_{23}	0.408										0.010
ν_{24}	0.458										-0.087

Table S4. On-diagonal quadratic (top) and bilinear (bottom) intra-state coupling constants $\gamma^{(i)}_{\alpha,\alpha}$ and $\gamma^{(i)}_{\alpha,\beta}$ determined by fitting the adiabatic PESs for all vibrational modes. Corresponding frequencies and single-point energies have been calculated at the (EOM-)CCSD/cc-pVDZ level of theory. The parameter highlighted in red has been altered to achieve a better correspondence with the experiment (cf. Tab. 5).

modes	$\gamma^{(i)}_{\alpha,\alpha}$ / eV				modes	$\gamma^{(i)}_{\alpha,\alpha}$ / eV			
	(1)	(2)	(3)	(4)		(1)	(2)	(3)	(4)
ν_1 , ν_1 †	0.004	-0.055	0.110	-0.001	ν_{13}, ν_{13}	0.025	0.012	0.013	-0.034
ν_2 , ν_2	0.033	0.004	-0.020	-0.032	ν_{14}, ν_{14}	0.020	0.018	0.021	0.022
ν_3 , ν_3	-0.014	-0.022	-0.003	-0.017	ν_{15}, ν_{15}	-0.005	-0.009	-0.010	-0.019
ν_4 , ν_4 †	0.042	0.030	0.089	0.065	ν_{16}, ν_{16}	-0.028	-0.015	-0.010	-0.009
ν_5 , ν_5	-0.011	-0.018	-0.005	-0.013	ν_{17}, ν_{17}	0.013	0.013	0.001	0.004
ν_6 , ν_6	0.019	0.016	0.007	0.020	ν_{18}, ν_{18}	-0.049	-0.030	-0.046	-0.014
ν_7 , ν_7	-0.002	-0.010	0.020	-0.008	ν_{19}, ν_{19} †	-0.010	-0.022	-0.010	-0.007
ν_8 , ν_8	0.005	0.001	0.009	0.004	ν_{20}, ν_{20}	-0.016	0.004	-0.008	-0.040
ν_9 , ν_9	-0.010	-0.047	-0.055	-0.079	ν_{21}, ν_{21} †	-0.049	-0.041	-0.035	-0.036
ν_{10}, ν_{10}	-0.009	-0.004	0.004	-0.021	ν_{22}, ν_{22} †	-0.009	-0.014	-0.004	0.000
ν_{11}, ν_{11} †	0.008	0.017	0.022	0.013	ν_{23}, ν_{23} †	0.006	-0.018	-0.017	0.031
ν_{12}, ν_{12}	-0.002	0.007	-0.009	0.011	ν_{24}, ν_{24} †	0.079	0.081	0.109	-0.112

modes	$\gamma^{(i)}_{\alpha,\beta}$ / eV				modes	$\gamma^{(i)}_{\alpha,\beta}$ / eV			
	(1)	(2)	(3)	(4)		(1)	(2)	(3)	(4)
ν_3 , ν_{23}	-0.001	0.000	0.000	-0.001	ν_{19}, ν_{24}	-0.002	-0.002	-0.002	0.002
ν_3 , ν_{24}	-0.001	0.002	0.002	0.002	ν_{21}, ν_{23}	-0.001	-0.001	-0.001	-0.001
ν_7 , ν_{24}	0.001	0.001	0.001	0.001	ν_{21}, ν_{24}	0.000	0.001	0.001	0.001
ν_{18}, ν_{23}	0.001	0.001	0.001	0.001	ν_{23}, ν_{24}	0.003	0.003	0.003	0.003
ν_{18}, ν_{24}	-0.001	-0.001	-0.001	-0.001					

† Corresponding parameters are replaced by higher order diabatic and Morse potentials (cf. Tab. S5 and S6).

Table S5. Diabatic quartic potential parameters $\gamma_\alpha^{(i)}$ and $\epsilon_\alpha^{(i)}$ determined by fitting the adiabatic PESs for the vibrational modes ν_1, ν_4 and ν_{22}. Corresponding frequencies and single-point energies have been calculated at the (EOM-)CCSD/cc-pVDZ level of theory.

modes		Parameters / eV				
		(0)	(1)	(2)	(3)	(4)
ν_1	$\gamma_\alpha^{(i)}$	0.009	0.004	0.003	0.027	-0.006
	$\epsilon_\alpha^{(i)}$	0.030	0.027	0.026	0.028	0.026
ν_4	$\gamma_\alpha^{(i)}$	0.064	0.042	0.030	0.089	0.065
	$\epsilon_\alpha^{(i)}$	0.160	0.163	0.194	0.122	0.129
ν_{22}	$\gamma_\alpha^{(i)}$	-0.011	-0.009	-0.014	-0.004	0.000
	$\epsilon_\alpha^{(i)}$	0.079	0.078	0.079	0.076	0.074

Table S6. Morse potential parameters $D_\alpha^{(i)}$, $\alpha_\alpha^{(i)}$ and $Q_{0,\alpha}^{(i)}$ determined by fitting the adiabatic PESs for the vibrational modes ν_{11}, ν_{19}, ν_{21}, ν_{23} and ν_{24}. Corresponding frequencies and single-point energies have been calculated at the (EOM-)CCSD/cc-pVDZ level of theory.

modes		Parameters				
		(0)	(1)	(2)	(3)	(4)
ν_{11}	$D_\alpha^{(i)}$ / eV	7.490	8.013	8.471	9.422	8.611
	$\alpha_\alpha^{(i)}$	0.087	0.088	0.088	0.085	0.086
	$Q_{0,\alpha}^{(i)}$	-0.274	-0.880	-0.982	-1.393	-0.808
ν_{19}	$D_\alpha^{(i)}$ / eV	98.999	98.999	98.998	98.998	98.997
	$\alpha_\alpha^{(i)}$	-0.032	-0.032	-0.030	-0.031	-0.031
	$Q_{0,\alpha}^{(i)}$	-0.374	-0.603	-1.035	-1.144	-1.439
ν_{21}	$D_\alpha^{(i)}$ / eV	98.999	98.998	98.997	99.000	98.998
	$\alpha_\alpha^{(i)}$	-0.034	-0.030	-0.031	-0.031	-0.031
	$Q_{0,\alpha}^{(i)}$	-0.150	-1.283	-1.819	-0.653	-1.430
ν_{23}	$D_\alpha^{(i)}$ / eV	8.847	8.927	7.017	7.017	10.631
	$\alpha_\alpha^{(i)}$	-0.152	-0.152	-0.166	-0.166	-0.144
	$Q_{0,\alpha}^{(i)}$	0.040	0.069	0.090	0.090	0.099
ν_{24}	$D_\alpha^{(i)}$ / eV	4.098	4.894	4.937	5.390	4.959
	$\alpha_\alpha^{(i)}$	0.277	0.232	0.233	0.229	0.186
	$Q_{0,\alpha}^{(i)}$	-0.534	-0.089	-0.231	-0.152	0.294

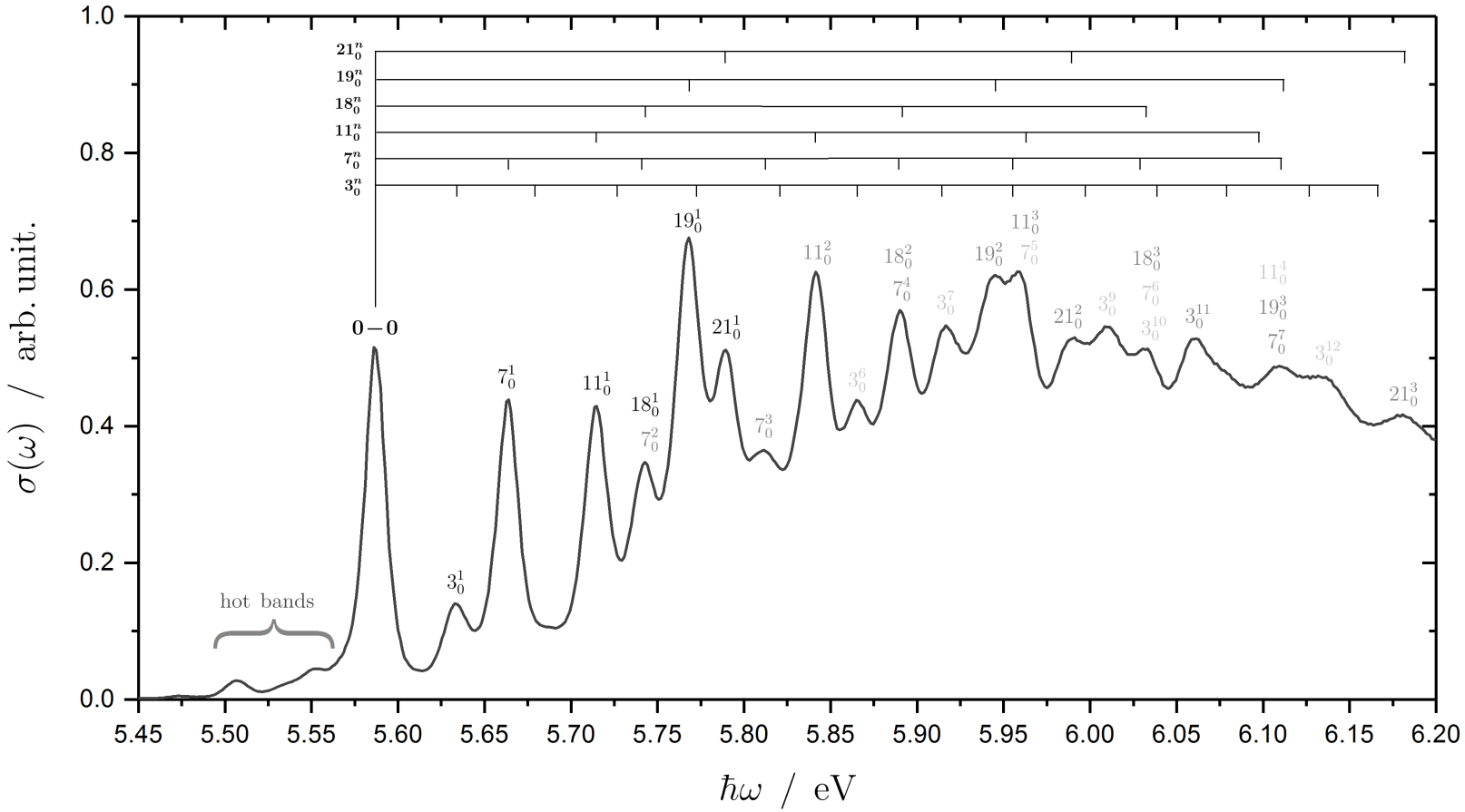

Figure S4. Experimental absorption spectra for the second excitation band of maleimide represented by the absorption cross section σ as a function of the photon energy $\hbar\omega$. The spectrum is shown for our vapour phase result at 315 K. A suggestion for the peak assignment of the most important vibronic excitations is given based on investigating the simulation results by employing the 6-mode model. The notation reads the a_1 vibrational mode followed by the excitation from the electronic and vibrational ground state (subscript) to the excited vibratrational state of the $2\,^1B_2$ electronic state (superscript). All peaks are assigned relative to the 0–0 transition.

```
#-------------------------------------------
# Maleimide VCHam
#-------------------------------------------

RUN-SECTION
    name = fromS3
    propagate
    tfinal = 200 tout=0.5 tpsi=5.0
    output gridpop=el psi auto=twice
END-RUN-SECTION

OPERATOR-SECTION
    opname = maleimide
END-OPERATOR-SECTION

SPF-BASIS-SECTION
    multi-set
    v7,v18  = 2,2,35,32,5
    v1,v11  = 2,2,35,32,5
    v4,v19  = 2,2,18,18,4
END-SPF-BASIS-SECTION

PRIMITIVE-BASIS-SECTION
    el      el      5
    v1      HO      16      0.00      1.00      1.00
    v2      HO      11      0.00      1.00      1.00
    v3      HO      21      0.00      1.00      1.00
    v4      HO      16      0.00      1.00      1.00
    v5      HO      11      0.00      1.00      1.00
    v6      HO      11      0.00      1.00      1.00
    v7      HO      21      0.00      1.00      1.00
    v8      HO      11      0.00      1.00      1.00
    v9      HO      21      0.00      1.00      1.00
    v10     HO      10      0.00      1.00      1.00
    v11     HO      16      0.00      1.00      1.00
    v12     HO      11      0.00      1.00      1.00
    v13     HO      11      0.00      1.00      1.00
    v14     HO      11      0.00      1.00      1.00
    v15     HO      11      0.00      1.00      1.00
    v16     HO      11      0.00      1.00      1.00
    v17     HO      11      0.00      1.00      1.00
    v18     HO      31      0.00      1.00      1.00
    v19     HO      16      0.00      1.00      1.00
    v20     HO      11      0.00      1.00      1.00
    v21     HO      16      0.00      1.00      1.00
    v22     HO      11      0.00      1.00      1.00
    v23     HO      11      0.00      1.00      1.00
    v24     HO      11      0.00      1.00      1.00
end-primitive-basis-section

INIT_WF-SECTION
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    init_state =  4
    v1      HO      0.00    0.00      1.00      1.00
    v2      HO      0.00    0.00      1.00      1.00
    v3      HO      0.00    0.00      1.00      1.00
    v4      HO      0.00    0.00      1.00      1.00
    v5      HO      0.00    0.00      1.00      1.00
    v6      HO      0.00    0.00      1.00      1.00
    v7      HO      0.00    0.00      1.00      1.00
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61      v8      HO      0.00    0.00    1.00    1.00
62      v9      HO      0.00    0.00    1.00    1.00
63      v10     HO      0.00    0.00    1.00    1.00
64      v11     HO      0.00    0.00    1.00    1.00
65      v12     HO      0.00    0.00    1.00    1.00
66      v13     HO      0.00    0.00    1.00    1.00
67      v14     HO      0.00    0.00    1.00    1.00
68      v15     HO      0.00    0.00    1.00    1.00
69      v16     HO      0.00    0.00    1.00    1.00
70      v17     HO      0.00    0.00    1.00    1.00
71      v18     HO      0.00    0.00    1.00    1.00
72      v19     HO      0.00    0.00    1.00    1.00
73      v20     HO      0.00    0.00    1.00    1.00
74      v21     HO      0.00    0.00    1.00    1.00
75      v22     HO      0.00    0.00    1.00    1.00
76      v23     HO      0.00    0.00    1.00    1.00
77      v24     HO      0.00    0.00    1.00    1.00
78      end-build
79  END-INIT_WF-SECTION
80
81  END-INPUT
```

```
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Maleimide VCHam model.
Energies SA(11)-CASPT2(12,9)/cc-pVDZ  Other parameters  EOM-CCSD/cc-pVDZ.
END-TITLE
END-OP_DEFINE-SECTION

PARAMETER-SECTION

#Frequencies

omega_1         =    0.01401  , ev
omega_2         =    0.03583  , ev
omega_3         =    0.04917  , ev
omega_4         =    0.06180  , ev
omega_5         =    0.06709  , ev
omega_6         =    0.07921  , ev
omega_7         =    0.07960  , ev
omega_8         =    0.08424  , ev
omega_9         =    0.09654  , ev
omega_10        =    0.10525  , ev
omega_11        =    0.11441  , ev
omega_12        =    0.11549  , ev
omega_13        =    0.11886  , ev
omega_14        =    0.13270  , ev
omega_15        =    0.14491  , ev
omega_16        =    0.16680  , ev
omega_17        =    0.16951  , ev
omega_18        =    0.17204  , ev
omega_19        =    0.20630  , ev
omega_20        =    0.23199  , ev
omega_21        =    0.23661  , ev
omega_22        =    0.40491  , ev
omega_23        =    0.40773  , ev
omega_24        =    0.45788  , ev

#Energies

E1              =    0.00000  , ev
E2              =    3.37000  , ev
E3              =    3.96000  , ev
E4              =    4.62000  , ev
E5              =    5.80000  , ev

#On-Diagonal Linear Coupling Constants (Kappa)

kappa2_3        =   -0.04397  , ev
kappa2_7        =   -0.04125  , ev
kappa2_11       =    0.06880  , ev
kappa2_14       =   -0.03806  , ev
kappa2_18       =    0.18713  , ev
kappa2_19       =    0.04920  , ev
kappa2_21       =    0.22930  , ev
kappa2_23       =   -0.01190  , ev
kappa2_24       =   -0.00570  , ev
kappa3_3        =    0.02012  , ev
kappa3_7        =   -0.06468  , ev
kappa3_11       =    0.08920  , ev
kappa3_14       =   -0.03719  , ev
kappa3_18       =    0.08324  , ev
```

```
kappa3_19       =   0.13040 , ev
kappa3_21       =   0.35950 , ev
kappa3_23       =  -0.01350 , ev
kappa3_24       =   0.00720 , ev
kappa4_3        =  -0.05391 , ev
kappa4_7        =  -0.15750 , ev
kappa4_11       =   0.12700 , ev
kappa4_14       =  -0.05000 , ev
kappa4_18       =   0.35229 , ev
kappa4_19       =   0.16880 , ev
kappa4_21       =   0.10010 , ev
kappa4_23       =  -0.01330 , ev
kappa4_24       =  -0.04360 , ev
kappa5_3        =  -0.00597 , ev
kappa5_7        =  -0.10000 , ev
kappa5_11       =   0.06450 , ev
kappa5_14       =  -0.08558 , ev
kappa5_18       =   0.10946 , ev
kappa5_19       =   0.22870 , ev
kappa5_21       =   0.27890 , ev
kappa5_23       =  -0.02710 , ev
kappa5_24       =  -0.01010 , ev

#Off-Diagonal Linear Coupling Constants (Lambda)

lambda1_2_1     =  -0.01111 , ev
lambda1_2_4     =   0.03901 , ev
lambda1_2_6     =  -0.02279 , ev
lambda1_2_10    =  -0.03680 , ev
lambda1_3_2     =  -0.01111 , ev
lambda1_3_4     =  -0.13100 , ev
lambda1_3_9     =   0.01203 , ev
lambda1_3_13    =  -0.03389 , ev
lambda1_4_5     =   0.00080 , ev
lambda1_4_8     =  -0.01106 , ev
lambda1_4_12    =  -0.00873 , ev
lambda1_4_15    =   0.01329 , ev
lambda1_4_16    =  -0.01881 , ev
lambda1_4_17    =   0.00791 , ev
lambda1_4_20    =   0.04713 , ev
lambda1_4_22    =  -0.00181 , ev
lambda1_5_5     =  -0.00520 , ev
lambda1_5_8     =   0.01673 , ev
lambda1_5_12    =   0.01221 , ev
lambda1_5_15    =   0.00287 , ev
lambda1_5_16    =  -0.00610 , ev
lambda1_5_17    =   0.00119 , ev
lambda1_5_20    =  -0.10908 , ev
lambda1_5_22    =   0.00131 , ev
lambda2_3_5     =   0.02252 , ev
lambda2_3_8     =   0.02779 , ev
lambda2_3_12    =   0.00515 , ev
lambda2_3_15    =   0.04166 , ev
lambda2_3_16    =  -0.03613 , ev
lambda2_3_17    =   0.03490 , ev
lambda2_3_20    =  -0.17187 , ev
lambda2_3_22    =  -0.01259 , ev
lambda2_4_2     =   0.05457 , ev
lambda2_4_9     =   0.11012 , ev
lambda2_4_13    =   0.04018 , ev
```

```
lambda2_5_2     =  -0.12086 , ev
lambda2_5_9     =   0.13761 , ev
lambda2_5_13    =   0.16415 , ev
lambda3_4_4     =   0.08981 , ev
lambda3_4_6     =   0.00490 , ev
lambda3_4_10    =  -0.00962 , ev
lambda3_5_1     =  -0.00051 , ev
lambda3_5_4     =  -0.07613 , ev
lambda3_5_6     =   0.03467 , ev
lambda3_5_10    =  -0.07513 , ev
lambda4_5_3     =  -0.10000 , ev
lambda4_5_7     =  -0.08929 , ev
lambda4_5_11    =   0.04827 , ev
lambda4_5_14    =  -0.00241 , ev
lambda4_5_18    =   0.07127 , ev
lambda4_5_19    =  -0.02844 , ev
lambda4_5_21    =  -0.02934 , ev
lambda4_5_23    =   0.00950 , ev
lambda4_5_24    =  -0.08733 , ev

#On-Diagonal Bilinear Coupling Constants (Gamma)

gamma2_2_2      =   0.03292 , ev
gamma2_3_3      =  -0.01433 , ev
gamma2_3_23     =  -0.00050 , ev
gamma2_3_24     =   0.00140 , ev
gamma2_5_5      =  -0.01096 , ev
gamma2_6_6      =   0.01850 , ev
gamma2_7_7      =  -0.00239 , ev
gamma2_7_23     =  -0.00020 , ev
gamma2_7_24     =   0.00050 , ev
gamma2_8_8      =   0.00472 , ev
gamma2_9_9      =  -0.00979 , ev
gamma2_10_10    =  -0.00934 , ev
gamma2_12_12    =  -0.00175 , ev
gamma2_13_13    =   0.02519 , ev
gamma2_14_14    =   0.02017 , ev
gamma2_15_15    =  -0.00516 , ev
gamma2_16_16    =  -0.02775 , ev
gamma2_17_17    =   0.01250 , ev
gamma2_18_18    =  -0.04933 , ev
gamma2_18_19    =  -0.00010 , ev
gamma2_18_23    =   0.00050 , ev
gamma2_18_24    =  -0.00080 , ev
gamma2_19_23    =  -0.00010 , ev
gamma2_19_24    =  -0.00180 , ev
gamma2_20_20    =  -0.01565 , ev
gamma2_21_23    =  -0.00090 , ev
gamma2_21_24    =   0.00040 , ev
gamma2_23_23    =   0.12380 , ev
gamma2_23_24    =   0.00250 , ev
gamma2_24_24    =   0.37860 , ev
gamma3_2_2      =   0.00366 , ev
gamma3_3_3      =  -0.02179 , ev
gamma3_3_23     =  -0.00050 , ev
gamma3_3_24     =   0.00150 , ev
gamma3_5_5      =  -0.01828 , ev
gamma3_6_6      =   0.01583 , ev
gamma3_7_7      =  -0.00976 , ev
gamma3_7_23     =  -0.00020 , ev
```

```
gamma3_7_24     =    0.00050 , ev
gamma3_8_8      =    0.00058 , ev
gamma3_9_9      =   -0.04715 , ev
gamma3_10_10    =   -0.00375 , ev
gamma3_12_12    =    0.00657 , ev
gamma3_13_13    =    0.01187 , ev
gamma3_14_14    =    0.01815 , ev
gamma3_15_15    =   -0.00938 , ev
gamma3_16_16    =   -0.01457 , ev
gamma3_17_17    =    0.01265 , ev
gamma3_18_18    =   -0.03003 , ev
gamma3_18_23    =    0.00050 , ev
gamma3_18_24    =   -0.00080 , ev
gamma3_19_24    =   -0.00180 , ev
gamma3_20_20    =    0.00397 , ev
gamma3_21_23    =   -0.00090 , ev
gamma3_21_24    =    0.00060 , ev
gamma3_23_23    =    0.14090 , ev
gamma3_23_24    =    0.00250 , ev
gamma3_24_24    =    0.37960 , ev
gamma4_1_4      =   -0.00010 , ev
gamma4_2_2      =   -0.02038 , ev
gamma4_3_3      =   -0.00285 , ev
gamma4_3_23     =   -0.00040 , ev
gamma4_3_24     =    0.00160 , ev
gamma4_5_5      =   -0.00540 , ev
gamma4_6_6      =    0.00702 , ev
gamma4_7_7      =    0.02001 , ev
gamma4_7_21     =    0.00010 , ev
gamma4_7_23     =   -0.00030 , ev
gamma4_7_24     =    0.00080 , ev
gamma4_8_8      =    0.00868 , ev
gamma4_9_9      =   -0.05547 , ev
gamma4_10_10    =    0.00350 , ev
gamma4_12_12    =   -0.00889 , ev
gamma4_13_13    =    0.01293 , ev
gamma4_14_14    =    0.02123 , ev
gamma4_15_15    =   -0.00973 , ev
gamma4_16_16    =   -0.00976 , ev
gamma4_17_17    =    0.00067 , ev
gamma4_18_18    =   -0.04629 , ev
gamma4_18_21    =   -0.00030 , ev
gamma4_18_23    =    0.00050 , ev
gamma4_18_24    =   -0.00090 , ev
gamma4_19_21    =    0.00020 , ev
gamma4_19_23    =    0.00030 , ev
gamma4_19_24    =   -0.00190 , ev
gamma4_20_20    =   -0.00813 , ev
gamma4_21_23    =   -0.00090 , ev
gamma4_21_24    =    0.00050 , ev
gamma4_23_23    =    0.18860 , ev
gamma4_23_24    =    0.00250 , ev
gamma4_24_24    =    0.41440 , ev
gamma5_2_2      =   -0.03203 , ev
gamma5_3_3      =   -0.01742 , ev
gamma5_3_21     =    0.00010 , ev
gamma5_3_23     =   -0.00050 , ev
gamma5_3_24     =    0.00160 , ev
gamma5_5_5      =   -0.01297 , ev
gamma5_6_6      =    0.02032 , ev
```

```
gamma5_7_7      =  -0.00827  , ev
gamma5_7_19     =   0.00020  , ev
gamma5_7_23     =  -0.00030  , ev
gamma5_7_24     =   0.00070  , ev
gamma5_8_8      =   0.00365  , ev
gamma5_9_9      =  -0.07860  , ev
gamma5_10_10    =  -0.02081  , ev
gamma5_12_12    =  -0.01105  , ev
gamma5_13_13    =  -0.03406  , ev
gamma5_14_14    =   0.02246  , ev
gamma5_15_15    =  -0.01948  , ev
gamma5_16_16    =  -0.00925  , ev
gamma5_17_17    =   0.00384  , ev
gamma5_18_18    =  -0.02000  , ev
gamma5_18_19    =  -0.00010  , ev
gamma5_18_21    =  -0.00020  , ev
gamma5_18_23    =   0.00050  , ev
gamma5_18_24    =  -0.00090  , ev
gamma5_19_23    =  -0.00010  , ev
gamma5_19_24    =  -0.00180  , ev
gamma5_20_20    =  -0.03978  , ev
gamma5_21_23    =  -0.00100  , ev
gamma5_21_24    =   0.00060  , ev
gamma5_23_23    =   0.14800  , ev
gamma5_23_24    =   0.00260  , ev
gamma5_24_24    =   0.32680  , ev

# Diabatic Curves with Parameters

1EPm1       =    0.02953750  , ev
1GAm1       =    0.00932715  , ev
2EPm1       =    0.02669442  , ev
2GAm1       =    0.00424668  , ev
3EPm1       =    0.02580022  , ev
3GAm1       =    0.00303797  , ev
4EPm1       =    0.02777598  , ev
4GAm1       =    0.02667294  , ev
5EPm1       =    0.02646936  , ev
5GAm1       =   -0.00568607  , ev
1EPm4       =    0.16044840  , ev
1GAm4       =    0.06389122  , ev
2EPm4       =    0.16335388  , ev
2GAm4       =    0.04196290  , ev
3EPm4       =    0.19406492  , ev
3GAm4       =    0.02985938  , ev
4EPm4       =    0.12221038  , ev
4GAm4       =    0.08889845  , ev
5EPm4       =    0.12922395  , ev
5GAm4       =    0.06460660  , ev
1D_11       =    7.49022084  , ev
1A_11       =    0.08740201
1X_11       =   -0.27403853
1E_11       =    0.00000000
2D_11       =    8.01298486  , ev
2A_11       =    0.08749234
2X_11       =   -0.87974735
2E_11       =    0.00000000
3D_11       =    8.47057780  , ev
3A_11       =    0.08788952
3X_11       =   -0.98169116
```

```
3E_11       =     0.00000000
4D_11       =     9.42188428 , ev
4A_11       =     0.08491312
4X_11       =    -1.39264070
4E_11       =     0.00000000
5D_11       =     8.61069021 , ev
5A_11       =     0.08613512
5X_11       =    -1.10000000
5E_11       =     0.00000000
1D_19       =    98.99896190 , ev
1A_19       =    -0.03229799
1X_19       =    -0.37352548
1E_19       =     0.00000000
2D_19       =    98.99894596 , ev
2A_19       =    -0.03150321
2X_19       =    -0.60265617
2E_19       =     0.00000000
3D_19       =    98.99889264 , ev
3A_19       =    -0.03054705
3X_19       =    -1.03500346
3E_19       =     0.00000000
4D_19       =    98.99894499 , ev
4A_19       =    -0.03148955
4X_19       =    -1.14453090
4E_19       =     0.00000000
5D_19       =    98.99796281 , ev
5A_19       =    -0.03000000
5X_19       =    -1.43979206
5E_19       =     0.00000000
1D_21       =    98.99998223 , ev
1A_21       =    -0.03393087
1X_21       =    -0.14964156
1E_21       =     0.00000000
2D_21       =    98.99898909 , ev
2A_21       =    -0.03080050
2X_21       =    -1.28335964
2E_21       =     0.00000000
3D_21       =    98.99798507 , ev
3A_21       =    -0.03140394
3X_21       =    -1.81955451
3E_21       =     0.00000000
4D_21       =    99.00099674 , ev
4A_21       =    -0.03189363
4X_21       =    -0.65315449
4E_21       =     0.00000000
5D_21       =    98.99898221 , ev
5A_21       =    -0.03180336
5X_21       =    -1.20000000
5E_21       =     0.00000000
1EPm22      =     0.07905662 , ev
1GAm22      =    -0.01111726 , ev
2EPm22      =     0.07849771 , ev
2GAm22      =    -0.00914977 , ev
3EPm22      =     0.07912041 , ev
3GAm22      =    -0.01457494 , ev
4EPm22      =     0.07611320 , ev
4GAm22      =    -0.00407954 , ev
5EPm22      =     0.07402383 , ev
5GAm22      =     0.00036484 , ev
1D_23       =     8.84700741 , ev
```

```
1A_23       =    -0.15210754
1X_23       =     0.04040257
1E_23       =     0.00000000
2D_23       =     8.92723004 , ev
2A_23       =    -0.15227466
2X_23       =     0.06917546
2E_23       =     0.00000000
3D_23       =     7.01717240 , ev
3A_23       =    -0.16660540
3X_23       =     0.09089346
3E_23       =     0.00000000
4D_23       =     7.01783796 , ev
4A_23       =    -0.16677994
4X_23       =     0.09015606
4E_23       =     0.00000000
5D_23       =    10.63103976 , ev
5A_23       =    -0.14367132
5X_23       =     0.09923984
5E_23       =     0.00000000
1D_24       =     4.09820678 , ev
1A_24       =     0.27737724
1X_24       =    -0.53445499
1E_24       =     0.00000000
2D_24       =     4.89403508 , ev
2A_24       =     0.23235153
2X_24       =    -0.08894778
2E_24       =     0.00000000
3D_24       =     4.93739020 , ev
3A_24       =     0.23351534
3X_24       =    -0.23151132
3E_24       =     0.00000000
4D_24       =     5.39001484 , ev
4A_24       =     0.22928893
4X_24       =    -0.15237473
4E_24       =     0.00000000
5D_24       =     4.95930645 , ev
5A_24       =     0.18665039
5X_24       =     0.29467437
5E_24       =     0.00000000

end-parameter-section

LABELS-SECTION

# Diabatic Function Labels

v1m11=morse1[1D_11,1A_11,1X_11,1E_11]
v2m11=morse1[2D_11,2A_11,2X_11,2E_11]
v3m11=morse1[3D_11,3A_11,3X_11,3E_11]
v4m11=morse1[4D_11,4A_11,4X_11,4E_11]
v5m11=morse1[5D_11,5A_11,5X_11,5E_11]
v1m19=morse1[1D_19,1A_19,1X_19,1E_19]
v2m19=morse1[2D_19,2A_19,2X_19,2E_19]
v3m19=morse1[3D_19,3A_19,3X_19,3E_19]
v4m19=morse1[4D_19,4A_19,4X_19,4E_19]
v5m19=morse1[5D_19,5A_19,5X_19,5E_19]
v1m21=morse1[1D_21,1A_21,1X_21,1E_21]
v2m21=morse1[2D_21,2A_21,2X_21,2E_21]
v3m21=morse1[3D_21,3A_21,3X_21,3E_21]
v4m21=morse1[4D_21,4A_21,4X_21,4E_21]
```

```
v5m21=morse1[5D_21,5A_21,5X_21,5E_21]
v1m23=morse1[1D_23,1A_23,1X_23,1E_23]
v2m23=morse1[2D_23,2A_23,2X_23,2E_23]
v3m23=morse1[3D_23,3A_23,3X_23,3E_23]
v4m23=morse1[4D_23,4A_23,4X_23,4E_23]
v5m23=morse1[5D_23,5A_23,5X_23,5E_23]
v1m24=morse1[1D_24,1A_24,1X_24,1E_24]
v2m24=morse1[2D_24,2A_24,2X_24,2E_24]
v3m24=morse1[3D_24,3A_24,3X_24,3E_24]
v4m24=morse1[4D_24,4A_24,4X_24,4E_24]
v5m24=morse1[5D_24,5A_24,5X_24,5E_24]

end-labels-section

HAMILTONIAN-SECTION

-----------------------------------------------------
modes| v1  | v2  | v3  | v4  | v5  | v6  | v7  | v8  | v9  | v10 |
modes| v11 | v12 | v13 | v14 | v15 | v16 | v17 | v18 | v19 | v20 |
modes| v21 | v22 | v23 | v24 | el
-----------------------------------------------------

# Kinetic Energy

omega_1             |1      KE
omega_2             |2      KE
omega_3             |3      KE
omega_4             |4      KE
omega_5             |5      KE
omega_6             |6      KE
omega_7             |7      KE
omega_8             |8      KE
omega_9             |9      KE
omega_10            |10     KE
omega_11            |11     KE
omega_12            |12     KE
omega_13            |13     KE
omega_14            |14     KE
omega_15            |15     KE
omega_16            |16     KE
omega_17            |17     KE
omega_18            |18     KE
omega_19            |19     KE
omega_20            |20     KE
omega_21            |21     KE
omega_22            |22     KE
omega_23            |23     KE
omega_24            |24     KE

# Potential for Harmonic Oscillator

0.5*omega_1         |1      q^2
0.5*omega_2         |2      q^2
0.5*omega_3         |3      q^2
0.5*omega_4         |4      q^2
0.5*omega_5         |5      q^2
0.5*omega_6         |6      q^2
0.5*omega_7         |7      q^2
0.5*omega_8         |8      q^2
0.5*omega_9         |9      q^2
```

```
0.5*omega_10        |10    q^2
0.5*omega_12        |12    q^2
0.5*omega_13        |13    q^2
0.5*omega_14        |14    q^2
0.5*omega_15        |15    q^2
0.5*omega_16        |16    q^2
0.5*omega_17        |17    q^2
0.5*omega_18        |18    q^2
0.5*omega_20        |20    q^2
0.5*omega_22        |22    q^2

# Electronic States

E1                                      |25     S1&1
E2                                      |25     S2&2
E3                                      |25     S3&3
E4                                      |25     S4&4
E5                                      |25     S5&5

# Lambda

lambda1_2_1         |1     q              |25     S1&2
lambda3_5_1         |1     q              |25     S3&5
lambda1_3_2         |2     q              |25     S1&3
lambda2_4_2         |2     q              |25     S2&4
lambda2_5_2         |2     q              |25     S2&5
lambda4_5_3         |3     q              |25     S4&5
lambda1_2_4         |4     q              |25     S1&2
lambda3_4_4         |4     q              |25     S3&4
lambda3_4_1         |1     q              |25     S3&4
lambda3_5_4         |4     q              |25     S3&5
lambda1_4_5         |5     q              |25     S1&4
lambda1_5_5         |5     q              |25     S1&5
lambda2_3_5         |5     q              |25     S2&3
lambda1_2_6         |6     q              |25     S1&2
lambda3_4_6         |6     q              |25     S3&4
lambda3_5_6         |6     q              |25     S3&5
lambda4_5_7         |7     q              |25     S4&5
lambda1_4_8         |8     q              |25     S1&4
lambda1_5_8         |8     q              |25     S1&5
lambda2_3_8         |8     q              |25     S2&3
lambda1_3_9         |9     q              |25     S1&3
lambda2_4_9         |9     q              |25     S2&4
lambda2_5_9         |9     q              |25     S2&5
lambda1_2_10        |10    q              |25     S1&2
lambda3_4_10        |10    q              |25     S3&4
lambda3_5_10        |10    q              |25     S3&5
lambda4_5_11        |11    q              |25     S4&5
lambda1_4_12        |12    q              |25     S1&4
lambda1_5_12        |12    q              |25     S1&5
lambda2_3_12        |12    q              |25     S2&3
lambda1_3_13        |13    q              |25     S1&3
lambda2_4_13        |13    q              |25     S2&4
lambda2_5_13        |13    q              |25     S2&5
lambda4_5_14        |14    q              |25     S4&5
lambda1_4_15        |15    q              |25     S1&4
lambda1_5_15        |15    q              |25     S1&5
lambda2_3_15        |15    q              |25     S2&3
lambda1_4_16        |16    q              |25     S1&4
lambda1_5_16        |16    q              |25     S1&5
```

```
lambda2_3_16          |16    q          |25    S2&3
lambda1_4_17          |17    q          |25    S1&4
lambda1_5_17          |17    q          |25    S1&5
lambda2_3_17          |17    q          |25    S2&3
lambda4_5_18          |18    q          |25    S4&5
lambda4_5_19          |19    q          |25    S4&5
lambda1_4_20          |20    q          |25    S1&4
lambda1_5_20          |20    q          |25    S1&5
lambda2_3_20          |20    q          |25    S2&3
lambda4_5_21          |21    q          |25    S4&5
lambda1_4_22          |22    q          |25    S1&4
lambda1_5_22          |22    q          |25    S1&5
lambda2_3_22          |22    q          |25    S2&3
lambda4_5_23          |23    q          |25    S4&5
lambda4_5_24          |24    q          |25    S4&5

# Kappa

kappa2_3              |3     q          |25    S2&2
kappa3_3              |3     q          |25    S3&3
kappa4_3              |3     q          |25    S4&4
kappa5_3              |3     q          |25    S5&5
kappa2_7              |7     q          |25    S2&2
kappa3_7              |7     q          |25    S3&3
kappa4_7              |7     q          |25    S4&4
kappa5_7              |7     q          |25    S5&5
kappa2_14             |14    q          |25    S2&2
kappa3_14             |14    q          |25    S3&3
kappa4_14             |14    q          |25    S4&4
kappa5_14             |14    q          |25    S5&5
kappa2_18             |18    q          |25    S2&2
kappa3_18             |18    q          |25    S3&3
kappa4_18             |18    q          |25    S4&4
kappa5_18             |18    q          |25    S5&5

# On-Diagonal Gamma Constants

0.5*gamma2_2_2        |2     q^2        |25    S2&2
0.5*gamma3_2_2        |2     q^2        |25    S3&3
0.5*gamma4_2_2        |2     q^2        |25    S4&4
0.5*gamma5_2_2        |2     q^2        |25    S5&5
0.5*gamma2_3_3        |3     q^2        |25    S2&2
0.5*gamma3_3_3        |3     q^2        |25    S3&3
0.5*gamma4_3_3        |3     q^2        |25    S4&4
0.5*gamma5_3_3        |3     q^2        |25    S5&5
0.5*gamma2_5_5        |5     q^2        |25    S2&2
0.5*gamma3_5_5        |5     q^2        |25    S3&3
0.5*gamma4_5_5        |5     q^2        |25    S4&4
0.5*gamma5_5_5        |5     q^2        |25    S5&5
0.5*gamma2_6_6        |6     q^2        |25    S2&2
0.5*gamma3_6_6        |6     q^2        |25    S3&3
0.5*gamma4_6_6        |6     q^2        |25    S4&4
0.5*gamma5_6_6        |6     q^2        |25    S5&5
0.5*gamma2_7_7        |7     q^2        |25    S2&2
0.5*gamma3_7_7        |7     q^2        |25    S3&3
0.5*gamma4_7_7        |7     q^2        |25    S4&4
0.5*gamma5_7_7        |7     q^2        |25    S5&5
0.5*gamma2_8_8        |8     q^2        |25    S2&2
0.5*gamma3_8_8        |8     q^2        |25    S3&3
0.5*gamma4_8_8        |8     q^2        |25    S4&4
```

```
0.5*gamma5_8_8          |8      q^2                     |25      S5&5
0.5*gamma2_9_9          |9      q^2                     |25      S2&2
0.5*gamma3_9_9          |9      q^2                     |25      S3&3
0.5*gamma4_9_9          |9      q^2                     |25      S4&4
0.5*gamma5_9_9          |9      q^2                     |25      S5&5
0.5*gamma2_10_10        |10     q^2                     |25      S2&2
0.5*gamma3_10_10        |10     q^2                     |25      S3&3
0.5*gamma4_10_10        |10     q^2                     |25      S4&4
0.5*gamma5_10_10        |10     q^2                     |25      S5&5
0.5*gamma2_12_12        |12     q^2                     |25      S2&2
0.5*gamma3_12_12        |12     q^2                     |25      S3&3
0.5*gamma4_12_12        |12     q^2                     |25      S4&4
0.5*gamma5_12_12        |12     q^2                     |25      S5&5
0.5*gamma2_13_13        |13     q^2                     |25      S2&2
0.5*gamma3_13_13        |13     q^2                     |25      S3&3
0.5*gamma4_13_13        |13     q^2                     |25      S4&4
0.5*gamma5_13_13        |13     q^2                     |25      S5&5
0.5*gamma2_14_14        |14     q^2                     |25      S2&2
0.5*gamma3_14_14        |14     q^2                     |25      S3&3
0.5*gamma4_14_14        |14     q^2                     |25      S4&4
0.5*gamma5_14_14        |14     q^2                     |25      S5&5
0.5*gamma2_15_15        |15     q^2                     |25      S2&2
0.5*gamma3_15_15        |15     q^2                     |25      S3&3
0.5*gamma4_15_15        |15     q^2                     |25      S4&4
0.5*gamma5_15_15        |15     q^2                     |25      S5&5
0.5*gamma2_16_16        |16     q^2                     |25      S2&2
0.5*gamma3_16_16        |16     q^2                     |25      S3&3
0.5*gamma4_16_16        |16     q^2                     |25      S4&4
0.5*gamma5_16_16        |16     q^2                     |25      S5&5
0.5*gamma2_17_17        |17     q^2                     |25      S2&2
0.5*gamma3_17_17        |17     q^2                     |25      S3&3
0.5*gamma4_17_17        |17     q^2                     |25      S4&4
0.5*gamma5_17_17        |17     q^2                     |25      S5&5
0.5*gamma2_18_18        |18     q^2                     |25      S2&2
0.5*gamma3_18_18        |18     q^2                     |25      S3&3
0.5*gamma4_18_18        |18     q^2                     |25      S4&4
0.5*gamma5_18_18        |18     q^2                     |25      S5&5
0.5*gamma2_20_20        |20     q^2                     |25      S2&2
0.5*gamma3_20_20        |20     q^2                     |25      S3&3
0.5*gamma4_20_20        |20     q^2                     |25      S4&4
0.5*gamma5_20_20        |20     q^2                     |25      S5&5

# Off-Diagonal Gamma Constants

gamma4_1_4              |1      q       |4      q       |25      S4&4
gamma5_3_21             |3      q       |21     q       |25      S5&5
gamma2_3_23             |3      q       |23     q       |25      S2&2
gamma3_3_23             |3      q       |23     q       |25      S3&3
gamma4_3_23             |3      q       |23     q       |25      S4&4
gamma5_3_23             |3      q       |23     q       |25      S5&5
gamma2_3_24             |3      q       |24     q       |25      S2&2
gamma3_3_24             |3      q       |24     q       |25      S3&3
gamma4_3_24             |3      q       |24     q       |25      S4&4
gamma5_3_24             |3      q       |24     q       |25      S5&5
gamma5_7_19             |7      q       |19     q       |25      S5&5
gamma4_7_21             |7      q       |21     q       |25      S4&4
gamma2_7_23             |7      q       |23     q       |25      S2&2
gamma3_7_23             |7      q       |23     q       |25      S3&3
gamma4_7_23             |7      q       |23     q       |25      S4&4
gamma5_7_23             |7      q       |23     q       |25      S5&5
```

```
gamma2_7_24          |7    q    |24   q    |25   S2&2
gamma3_7_24          |7    q    |24   q    |25   S3&3
gamma4_7_24          |7    q    |24   q    |25   S4&4
gamma5_7_24          |7    q    |24   q    |25   S5&5
gamma2_18_19         |18   q    |19   q    |25   S2&2
gamma5_18_19         |18   q    |19   q    |25   S5&5
gamma4_18_21         |18   q    |21   q    |25   S4&4
gamma5_18_21         |18   q    |21   q    |25   S5&5
gamma2_18_23         |18   q    |23   q    |25   S2&2
gamma3_18_23         |18   q    |23   q    |25   S3&3
gamma4_18_23         |18   q    |23   q    |25   S4&4
gamma5_18_23         |18   q    |23   q    |25   S5&5
gamma2_18_24         |18   q    |24   q    |25   S2&2
gamma3_18_24         |18   q    |24   q    |25   S3&3
gamma4_18_24         |18   q    |24   q    |25   S4&4
gamma5_18_24         |18   q    |24   q    |25   S5&5
gamma4_19_21         |19   q    |21   q    |25   S4&4
gamma2_19_23         |19   q    |23   q    |25   S2&2
gamma4_19_23         |19   q    |23   q    |25   S4&4
gamma5_19_23         |19   q    |23   q    |25   S5&5
gamma2_19_24         |19   q    |24   q    |25   S2&2
gamma3_19_24         |19   q    |24   q    |25   S3&3
gamma4_19_24         |19   q    |24   q    |25   S4&4
gamma5_19_24         |19   q    |24   q    |25   S5&5
gamma2_21_23         |21   q    |23   q    |25   S2&2
gamma3_21_23         |21   q    |23   q    |25   S3&3
gamma4_21_23         |21   q    |23   q    |25   S4&4
gamma5_21_23         |21   q    |23   q    |25   S5&5
gamma2_21_24         |21   q    |24   q    |25   S2&2
gamma3_21_24         |21   q    |24   q    |25   S3&3
gamma4_21_24         |21   q    |24   q    |25   S4&4
gamma5_21_24         |21   q    |24   q    |25   S5&5
gamma2_23_24         |23   q    |24   q    |25   S2&2
gamma3_23_24         |23   q    |24   q    |25   S3&3
gamma4_23_24         |23   q    |24   q    |25   S4&4
gamma5_23_24         |23   q    |24   q    |25   S5&5

# Morse/Anti-Morse Potential

1.0                  |11   v1m11            |25   S1&1
1.0                  |11   v2m11            |25   S2&2
1.0                  |11   v3m11            |25   S3&3
1.0                  |11   v4m11            |25   S4&4
1.0                  |11   v5m11            |25   S5&5
1.0                  |19   v1m19            |25   S1&1
1.0                  |19   v2m19            |25   S2&2
1.0                  |19   v3m19            |25   S3&3
1.0                  |19   v4m19            |25   S4&4
1.0                  |19   v5m19            |25   S5&5
1.0                  |21   v1m21            |25   S1&1
1.0                  |21   v2m21            |25   S2&2
1.0                  |21   v3m21            |25   S3&3
1.0                  |21   v4m21            |25   S4&4
1.0                  |21   v5m21            |25   S5&5
1.0                  |23   v1m23            |25   S1&1
1.0                  |23   v2m23            |25   S2&2
1.0                  |23   v3m23            |25   S3&3
1.0                  |23   v4m23            |25   S4&4
1.0                  |23   v5m23            |25   S5&5
1.0                  |24   v1m24            |25   S1&1
```

```
1.0                     |2 4    v2m24           |2 5    S2&2
1.0                     |2 4    v3m24           |2 5    S3&3
1.0                     |2 4    v4m24           |2 5    S4&4
1.0                     |2 4    v5m24           |2 5    S5&5

# Quartic Potential

0.041667*1EPm1          |1      q^4             |2 5    S1&1
0.50000*1GAm1           |1      q^2             |2 5    S1&1
0.041667*2EPm1          |1      q^4             |2 5    S2&2
0.50000*2GAm1           |1      q^2             |2 5    S2&2
0.041667*3EPm1          |1      q^4             |2 5    S3&3
0.50000*3GAm1           |1      q^2             |2 5    S3&3
0.041667*4EPm1          |1      q^4             |2 5    S4&4
0.50000*4GAm1           |1      q^2             |2 5    S4&4
0.041667*5EPm1          |1      q^4             |2 5    S5&5
0.50000*5GAm1           |1      q^2             |2 5    S5&5
0.041667*1EPm4          |4      q^4             |2 5    S1&1
0.50000*1GAm4           |4      q^2             |2 5    S1&1
0.041667*2EPm4          |4      q^4             |2 5    S2&2
0.50000*2GAm4           |4      q^2             |2 5    S2&2
0.041667*3EPm4          |4      q^4             |2 5    S3&3
0.50000*3GAm4           |4      q^2             |2 5    S3&3
0.041667*4EPm4          |4      q^4             |2 5    S4&4
0.50000*4GAm4           |4      q^2             |2 5    S4&4
0.041667*5EPm4          |4      q^4             |2 5    S5&5
0.50000*5GAm4           |4      q^2             |2 5    S5&5
0.041667*1EPm22         |2 2    q^4             |2 5    S1&1
0.50000*1GAm22          |2 2    q^2             |2 5    S1&1
0.041667*2EPm22         |2 2    q^4             |2 5    S2&2
0.50000*2GAm22          |2 2    q^2             |2 5    S2&2
0.041667*3EPm22         |2 2    q^4             |2 5    S3&3
0.50000*3GAm22          |2 2    q^2             |2 5    S3&3
0.041667*4EPm22         |2 2    q^4             |2 5    S4&4
0.50000*4GAm22          |2 2    q^2             |2 5    S4&4
0.041667*5EPm22         |2 2    q^4             |2 5    S5&5
0.50000*5GAm22          |2 2    q^2             |2 5    S5&5
END-HAMILTONIAN-SECTION

END-OPERATOR
```

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