Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials for Towards Accurate Prediction for Laser-Coolable Molecules: Relativistic Coupled-Cluster Calculations for Yttrium Monoxide and Prospects for Improving its Laser Cooling Efficiencies

The supplementary information includes a demonstration of the sensitivity of computed Franck-Condon factors (FCFs) with respect to harmonic frequencies (Table I) and Franck-Condon factors for a complete list of transitions between electronic states (Table II).

TABLE I. Calculated FCFs using Morse potentials with parameters obtained at the EOM-CCSD/∞Z/sc+ΔT level and with the use of various values for the harmonic frequency of the $X^2\Sigma$ state. The original EOM-CCSD/∞Z/sc+ΔT harmonic frequency for the $X^2\Sigma$ state is 853.5 cm^{-1}. As can be seen, a shift of harmonic frequencies by 50 cm^{-1} only changes individual computed FCFs by less than 1%.

		Harmonic frequencies for $X^2\Sigma$ state (cm^{-1})						
transitions	ν	803.5	823.5	843.5	853.5	863.5	883.5	903.5
$A^2\Pi(0) \rightarrow X^2\Sigma(\nu)$	0	99.699%	99.689%	99.665%	99.648%	99.627%	99.577%	99.515%
	1	0.295%	0.310%	0.326%	0.333%	0.340%	0.354%	0.368%
	2	0.006%	<0.001%	0.009%	0.019%	0.032%	0.069%	0.117%
$B^2\Sigma(0) \rightarrow X^2\Sigma(\nu)$	0	82.819%	82.552%	82.280%	82.142%	82.003%	81.724%	81.441%
	1	16.083%	16.129%	16.163%	16.176%	16.187%	16.202%	16.208%
	2	1.066%	1.265%	1.472%	1.579%	1.687%	1.909%	2.136%
	3	0.031%	0.053%	0.082%	0.098%	0.116%	0.155%	0.199%
	4	<0.001%	0.001%	0.003%	0.004%	0.006%	0.010%	0.015%
	5	<0.001%	<0.001%	<0.001%	<0.001%	<0.001%	<0.001%	0.001%
$A'^2\Delta(0) \rightarrow X^2\Sigma(\nu)$	0	87.448%	87.239%	87.023%	86.912%	86.800%	86.571%	86.338%
	1	12.061%	12.122%	12.174%	12.197%	12.218%	12.253%	12.281%
	2	0.485%	0.623%	0.773%	0.853%	0.934%	1.105%	1.284%
	3	0.006%	0.015%	0.029%	0.037%	0.046%	0.067%	0.092%
	4	<0.001%	<0.001%	0.001%	0.001%	0.002%	0.003%	0.005%

TABLE II. Calculated Franck-Condon factors using EOM-CCSD/∞Z/sc+ΔT+ΔSO ab initio potential energy surfaces.

transitions/ν	0	1	2	3	4	5
$A^2\Pi_{1/2}(0) \rightarrow X^2\Sigma_{1/2}(\nu)$	99.563%	0.416%	0.020%	<0.001%	<0.001%	<0.001%
$A^2\Pi_{3/2}(0) \rightarrow X^2\Sigma_{1/2}(\nu)$	99.687%	0.293%	0.019%	<0.001%	<0.001%	<0.001%
$A'^2\Delta_{3/2}(0) \rightarrow X^2\Sigma_{1/2}(\nu)$	86.600%	12.464%	0.895%	<0.040%	0.001%	<0.001%
$A'^2\Delta_{5/2}(0) \rightarrow X^2\Sigma_{1/2}(\nu)$	87.209%	11.936%	0.820%	<0.035%	0.001%	<0.001%
$B^2\Sigma_{1/2}(0) \rightarrow X^2\Sigma_{1/2}(\nu)$	82.411%	15.954%	1.536%	<0.094%	0.004%	<0.001%
$A^2\Pi_{1/2}(0) \rightarrow A'^2\Delta_{3/2}(\nu)$	90.762%	8.623%	0.580%	0.034%	0.002%	<0.001%
$A^2\Pi_{3/2}(0) \rightarrow A'^2\Delta_{3/2}(\nu)$	90.169%	9.139%	0.650%	0.040%	0.002%	<0.001%
$A^2\Pi_{1/2}(0) \rightarrow A'^2\Delta_{5/2}(\nu)$	91.279%	8.167%	0.523%	0.029%	0.001%	<0.001%
$A^2\Pi_{3/2}(0) \rightarrow A'^2\Delta_{5/2}(\nu)$	90.700%	8.675%	0.589%	0.034%	0.002%	<0.001%
$B^2\Sigma_{1/2}(0) \rightarrow A^2\Pi_{1/2}(\nu)$	87.118%	12.233%	0.633%	0.015%	<0.001%	<0.001%
$B^2\Sigma_{1/2}(0) \rightarrow A^2\Pi_{3/2}(\nu)$	86.443%	12.834%	0.706%	0.018%	<0.001%	<0.001%
$B^2\Sigma_{1/2}(0) \rightarrow A'^2\Delta_{3/2}(\nu)$	99.635%	0.365%	<0.001%	<0.001%	<0.001%	<0.001%
$B^2\Sigma_{1/2}(0) \rightarrow A'^2\Delta_{5/2}(\nu)$	99.514%	0.485%	0.001%	<0.001%	<0.001%	<0.001%