

## Supplementary Material

**Table 1** 9 geometric reference coordinates and 9 nonlinear parameters for three excited states

	$1^3A''$			$1^3A'$			$2^1A'$		
	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$
$\gamma_1^{(j)} / \alpha_0^{-1}$	0.4	0.8	0.8	0.6	1.1	1.1	2.0	1.0	1.0
$\gamma_2^{(j)} / \alpha_0^{-1}$	1.3	1.0	1.0	1.9	2.0	2.0	0.5	1.4	1.4
$\gamma_3^{(j)} / \alpha_0^{-1}$	0.7	0.6	0.6	0.5	0.5	0.5	0.2	0.7	0.7
$R_{1,\text{ref}}^{(j)} / \alpha_0$	5.0	4.0	4.0	2.0	5.0	5.0	2.0	5.0	5.0
$R_{2,\text{ref}}^{(j)} / \alpha_0$	3.0	3.0	3.0	3.0	3.0	4.0	4.0	4.0	4.0
$R_{3,\text{ref}}^{(j)} / \alpha_0$	5.0	3.0	3.0	5.0	2.5	2.5	5.0	5.0	5.0

**Table 2** 150 linear coefficients of  $1^3A''$  state

Coefficients	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$
$C_1/a_0^0$	0.1270721069	-0.0866997319	0.0126999242
$C_2/a_0^{-1}$	-0.0138029605	0.1070564802	-0.2009634644
$C_3/a_0^{-1}$	-0.1458595851	-0.0086054983	-0.0473640508
$C_4/a_0^{-2}$	-0.0116244092	0.0389554994	-0.0127787232
$C_5/a_0^{-2}$	0.0008031827	-0.0011487759	0.0327687688
$C_6/a_0^{-2}$	0.0219606283	-0.0244163656	-0.0239714433
$C_7/a_0^{-2}$	-0.0734572307	-0.0881194104	-0.0124604107
$C_8/a_0^{-3}$	-0.0322232727	0.0000882095	-0.0014502715
$C_9/a_0^{-3}$	0.0019515813	-0.0010833004	0.0021212340
$C_{10}/a_0^{-3}$	0.0037408155	-0.0012242468	-0.0037727714
$C_{11}/a_0^{-3}$	-0.0035350614	-0.0030937534	-0.0001958165
$C_{12}/a_0^{-3}$	-0.0019653374	0.0001181815	0.0044561897
$C_{13}/a_0^{-3}$	0.0021868348	-0.0044783403	-0.0012017187
$C_{14}/a_0^{-4}$	-0.0005492772	0.0007075458	-0.0023555748
$C_{15}/a_0^{-4}$	-0.0043644692	-0.0091085537	0.0053397610
$C_{16}/a_0^{-4}$	-0.0014153885	0.0002535352	0.0021026491
$C_{17}/a_0^{-4}$	0.0001390463	-0.0001413697	1.0074393851
$C_{18}/a_0^{-4}$	0.3055289149	0.4157788867	0.7265564411
$C_{19}/a_0^{-4}$	0.5728655976	0.4212240606	-0.2182001149

$C_{20}/a_0^{-4}$	0.1199964410	0.1455336100	0.0622636028
$C_{21}/a_0^{-4}$	0.4739083546	-0.0899036869	0.2254960970
$C_{22}/a_0^{-4}$	0.1389782677	0.1742362586	0.1061356633
$C_{23}/a_0^{-5}$	-0.0929283012	0.1541335943	-0.1269887985
$C_{24}/a_0^{-5}$	-0.0109408007	0.0206685516	-0.0865054606
$C_{25}/a_0^{-5}$	0.0003475608	0.0302479364	-0.0293526837
$C_{26}/a_0^{-5}$	-0.0101950207	0.0275752876	0.0573519943
$C_{27}/a_0^{-5}$	-0.0637195859	0.0064979995	-0.0275222760
$C_{28}/a_0^{-5}$	0.0031669257	0.0597574129	-0.0180981126
$C_{29}/a_0^{-5}$	0.0037809014	-0.0138671588	-0.0149524380
$C_{30}/a_0^{-5}$	0.0024793128	-0.0054938161	0.0034559352
$C_{31}/a_0^{-5}$	0.0033780868	0.0027476042	-0.0131912047
$C_{32}/a_0^{-5}$	0.0266901209	-0.0110793523	0.0120177122
$C_{33}/a_0^{-5}$	0.0121019164	0.0008124225	0.0038859592
$C_{34}/a_0^{-5}$	-0.0053599477	-2.6098340776	0.8562778550
$C_{35}/a_0^{-6}$	-4.0451324551	-0.2408268329	-1.5289613815
$C_{36}/a_0^{-6}$	0.9881079353	1.4646375495	0.2099649550
$C_{37}/a_0^{-6}$	0.1281343678	-0.2377806395	-0.4661687749
$C_{38}/a_0^{-6}$	-0.0690439180	-1.0854767606	-0.0016848069
$C_{39}/a_0^{-6}$	-0.0620243412	-0.1818672821	-0.0120281957
$C_{40}/a_0^{-6}$	0.1972922370	0.1110501712	-0.0220839263
$C_{41}/a_0^{-6}$	-0.0658809430	0.2074544129	0.0113442640
$C_{42}/a_0^{-6}$	0.0234080676	-0.0211092158	-0.0005513674
$C_{43}/a_0^{-6}$	-0.0239762431	0.0060465614	-0.0113953912
$C_{44}/a_0^{-6}$	0.0033057338	0.0010957308	0.0220907599
$C_{45}/a_0^{-6}$	-0.0377172936	0.0055885170	-0.0010197302
$C_{46}/a_0^{-6}$	0.0015419222	0.0006475648	-0.0009441139
$C_{47}/a_0^{-6}$	-0.0002024564	-0.0003667594	-0.0001401027
$C_{48}/a_0^{-6}$	0.0026810569	-0.0007552860	0.0002067691
$C_{49}/a_0^{-6}$	-0.0010234551	-0.0029940227	-0.0052644019
$C_{50}/a_0^{-6}$	-0.0028813990	-0.0021731194	0.0007890170

**Table 3** 150 linear coefficients of  $1^3A'$  state

Coefficients	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$
$C_1/a_0^0$	-0.1280101736	-0.0368487554	-0.0630109968
$C_2/a_0^{-1}$	-0.0560572316	-0.0575327328	0.0250159318
$C_3/a_0^{-1}$	-0.0085975812	-0.0145041570	-0.0033138403
$C_4/a_0^{-2}$	0.0004568096	-0.0158756471	-0.0002332552
$C_5/a_0^{-2}$	-0.0271608641	-0.0088618006	-0.0087699125
$C_6/a_0^{-2}$	-0.0153847156	0.0147944255	0.0005815977
$C_7/a_0^{-2}$	0.0124919586	-0.0123794709	0.0059347892
$C_8/a_0^{-3}$	0.0030363558	-0.0018814996	0.0000486472

$C_9/a_0^{-3}$	-0.0008874994	0.0076135697	-0.0016260035
$C_{10}/a_0^{-3}$	-0.0010678952	-0.0003992642	-0.0049185855
$C_{11}/a_0^{-3}$	0.0121297511	0.0053414908	0.0055171320
$C_{12}/a_0^{-3}$	0.0009381301	-0.0001466973	-0.0004258014
$C_{13}/a_0^{-3}$	0.0000415321	0.0016272963	0.0000178427
$C_{14}/a_0^{-4}$	-0.0006164771	-0.0002330745	0.0004246359
$C_{15}/a_0^{-4}$	-0.0012132501	-0.0023593314	0.0027634645
$C_{16}/a_0^{-4}$	0.0014227902	0.0007128384	0.0009401598
$C_{17}/a_0^{-4}$	-0.0000826338	-0.0003688401	-0.0068748209
$C_{18}/a_0^{-4}$	-0.0120752190	0.0110283818	-0.0235568119
$C_{19}/a_0^{-4}$	0.0114066537	0.0047258424	0.0098436457
$C_{20}/a_0^{-4}$	-0.0271386739	0.0174341050	0.0033072198
$C_{21}/a_0^{-4}$	0.0011663055	0.0261210778	-0.0023279861
$C_{22}/a_0^{-4}$	-0.0188932770	0.0085720744	-0.0138883353
$C_{23}/a_0^{-5}$	0.0103612548	0.0036980397	0.0252635952
$C_{24}/a_0^{-5}$	0.0107728156	-0.0062414155	-0.0086172353
$C_{25}/a_0^{-5}$	-0.0077590533	-0.0017867562	-0.0145922864
$C_{26}/a_0^{-5}$	0.0116965246	-0.0049795901	0.0055163452
$C_{27}/a_0^{-5}$	0.0143526951	0.0174614486	-0.0091441878
$C_{28}/a_0^{-5}$	-0.0111747071	0.0022369536	-0.0030438797
$C_{29}/a_0^{-5}$	-0.0010763077	-0.0016520682	-0.0038723900
$C_{30}/a_0^{-5}$	0.0040251695	-0.0022675673	-0.0001791827
$C_{31}/a_0^{-5}$	-0.0004083692	0.0009654301	0.0034966002
$C_{32}/a_0^{-5}$	0.0070809480	-0.0032298797	-0.0023945408
$C_{33}/a_0^{-5}$	0.0004735595	-0.0017600160	0.0007787468
$C_{34}/a_0^{-5}$	-0.0001874990	2.3039723719	0.2748679302
$C_{35}/a_0^{-6}$	-0.5353350868	0.1643535182	-0.0347001261
$C_{36}/a_0^{-6}$	0.2126307578	0.1108878803	0.0308226534
$C_{37}/a_0^{-6}$	0.0652550857	-0.0892837142	-0.0846438586
$C_{38}/a_0^{-6}$	-0.1365982492	-0.2176812565	-0.0027495660
$C_{39}/a_0^{-6}$	-0.0504268989	-0.0419112086	0.0138410788
$C_{40}/a_0^{-6}$	0.0226042646	0.0192638104	0.1192753758
$C_{41}/a_0^{-6}$	-0.0337355793	0.0399188618	-0.0001742452
$C_{42}/a_0^{-6}$	0.0011225676	0.0137591096	-0.0007257900
$C_{43}/a_0^{-6}$	-0.0038933976	0.0005033593	0.0014769713
$C_{44}/a_0^{-6}$	-0.0207962783	0.0094204601	-0.0089954531
$C_{45}/a_0^{-6}$	-0.0048292299	0.0050937672	0.0002995796
$C_{46}/a_0^{-6}$	-0.0003848672	-0.0004212585	-0.0003918450
$C_{47}/a_0^{-6}$	0.0006271773	0.0001939424	-0.0003236810
$C_{48}/a_0^{-6}$	0.0004915903	-0.0004841372	-0.0012048962
$C_{49}/a_0^{-6}$	-0.0010031261	0.0011316840	0.0013970664
$C_{50}/a_0^{-6}$	-0.0004931415	-0.0008294667	-0.0005766723

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Table 4 150 linear coefficients of  $2^1A'$  state

Coefficients	$P^{(1)}$	$P^{(2)}$	$P^{(3)}$
$C_1/a_0^0$	-0.0397016382	0.0142239429	-0.0398558247
$C_2/a_0^{-1}$	-0.0260308093	-0.0416386675	-0.0442248487
$C_3/a_0^{-1}$	0.0335920039	0.0079671315	-0.0217838952
$C_4/a_0^{-2}$	-0.0130896322	-0.0061226658	0.0177436783
$C_5/a_0^{-2}$	-0.0539975034	-0.0044557110	-0.0074580004
$C_6/a_0^{-2}$	-0.0246892513	-0.0034887170	-0.0014482422
$C_7/a_0^{-2}$	-0.0047754299	-0.0436451506	-0.0108771073
$C_8/a_0^{-3}$	0.0210433974	0.0011780209	-0.0014972606
$C_9/a_0^{-3}$	-0.0187990602	-0.0027063370	-0.0114901452
$C_{10}/a_0^{-3}$	0.0022003899	-0.0017662849	-0.0097056317
$C_{11}/a_0^{-3}$	-0.0110505384	0.0162250595	-0.0170798002
$C_{12}/a_0^{-3}$	0.0043407960	0.0001208796	0.0012359457
$C_{13}/a_0^{-3}$	-0.0048762489	-0.0011030971	-0.0057879428
$C_{14}/a_0^{-4}$	-0.0015200075	-0.0006028042	0.0002648752
$C_{15}/a_0^{-4}$	0.0002926224	-0.0005614396	-0.0028490910
$C_{16}/a_0^{-4}$	0.0052306161	-0.0081200164	0.0022048386
$C_{17}/a_0^{-4}$	-0.0032195094	0.0003864183	0.1826993331
$C_{18}/a_0^{-4}$	0.0294506073	-0.0111466920	0.0888660165
$C_{19}/a_0^{-4}$	0.1106405967	-0.1498966625	0.0526089288
$C_{20}/a_0^{-4}$	0.0059894166	0.0288843299	0.0018187545
$C_{21}/a_0^{-4}$	-0.0394138815	0.0049470995	-0.0098822129
$C_{22}/a_0^{-4}$	0.0081683870	0.0087725995	0.0174195129
$C_{23}/a_0^{-5}$	-0.0120753292	-0.0403207129	-0.0365245199
$C_{24}/a_0^{-5}$	-0.0060490209	0.0142094440	0.0323325642
$C_{25}/a_0^{-5}$	-0.0008676918	-0.0036527719	0.0018256282
$C_{26}/a_0^{-5}$	-0.0001257177	0.0018292216	-0.0058829370
$C_{27}/a_0^{-5}$	-0.0087925796	0.0016793432	0.0069218440
$C_{28}/a_0^{-5}$	0.0133923977	0.0010437298	0.0017575675
$C_{29}/a_0^{-5}$	0.0000962813	-0.0008209657	-0.0001865812
$C_{30}/a_0^{-5}$	0.0003840169	-0.0004346910	0.0006185679
$C_{31}/a_0^{-5}$	0.0000357008	-0.0008902042	-0.0014802088
$C_{32}/a_0^{-5}$	-0.0009177970	0.0015199225	0.0010783880
$C_{33}/a_0^{-5}$	0.0004951134	0.0007869384	0.0011841157
$C_{34}/a_0^{-5}$	0.0014310699	-0.0007886715	0.0050911099
$C_{35}/a_0^{-6}$	-0.0015029903	-0.0063115295	-0.0002167027
$C_{36}/a_0^{-6}$	0.0031187952	-0.0016222832	0.0019798092
$C_{37}/a_0^{-6}$	0.0015810248	-0.0001470928	-0.0039121034
$C_{38}/a_0^{-6}$	0.0011754428	0.0000663734	-0.0009776669
$C_{39}/a_0^{-6}$	-0.0002855216	0.0001763161	-0.0003651695
$C_{40}/a_0^{-6}$	0.0032484439	0.0006015936	-0.0001495835
$C_{41}/a_0^{-6}$	0.0002996202	0.0001690388	-0.0002322030
$C_{42}/a_0^{-6}$	0.0001772829	-0.0000407228	-0.0000336905

$C_{43}/a_0^{-6}$	0.0000413484	0.0000419088	0.0001847939
$C_{44}/a_0^{-6}$	-0.0001847005	0.0001628312	-0.0001252095
$C_{45}/a_0^{-6}$	-0.0000641009	0.0000384508	-0.0001078951
$C_{46}/a_0^{-6}$	-0.0000765787	0.0000347741	0.0001226817
$C_{47}/a_0^{-6}$	0.0000084668	-0.0000087134	0.0000071006
$C_{48}/a_0^{-6}$	0.0003989773	0.0002266374	-0.0001350852
$C_{49}/a_0^{-6}$	-0.0000784113	-0.0000907150	0.0000194969
$C_{50}/a_0^{-6}$	0.0000086382	-0.0000294080	-0.0000071673

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