Supplementary Material

Spin-orbit coupling in low-lying electronic states of CuH

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Table S1

Calculated spectroscopic constants (in cm^{-1}) for the ground and excited Ω states of CuH using an active space of 11 electrons in 7 orbitals. Experimental values are from references [8] and [17].

State (Ω)	Composition at r = 1.46 (Å)	r_e (Å)	T_e (cm^{-1})	D_e (cm^{-1})	ω_e (cm^{-1})	v_{0-0} (cm^{-1})	$\Delta G_{1/2}$ (cm^{-1})	B_e (cm^{-1})
0^+ (I)	$X^1\Sigma^+$ (100)	1.459	0	21531	1927	0	1850	7.984
Exp. 0^+(I)	**$X^1\Sigma^+$**	**1.463**	**0**	**22980**	**1941**	**0**	**1866.41**	**7.945**
0^- (I)	$1^3\Sigma^+$ (98)+ $1^3\Pi$ (2)	1.519	18313	3218	1832	18254	1741	7.365
1(I)	$1^3\Sigma^+$ (99) + $1^1\Pi$ (1)	1.519	18328	3203	1834	18269	1743	7.365
0^+ (II)	$A^1\Sigma^+$ (94)+ $1^3\Pi$ (6)	1.556	21889	11204	1757	21795	1673	7.019
Exp. 0^+(II)	**$A^1\Sigma^+$**	**1.572**	**23434.2**	**10748**	**1698**	**23311.1**	**1610.4**	**6.874**
2(I)	$1^3\Pi$ (87) +$1^3\Delta$ (12) +$1^1\Delta$ (1)	1.604	23314	9812	1689	23183	1610	6.605
1(II)	$1^3\Pi$ (80) +$1^1\Pi$ (6) +$1^3\Delta$ (14)	1.604	23691	9441	1685	23558	1604	6.605
3(I)	$1^3\Delta$ (100)	1.591	24084	9042	1653	23931	1557	6.714
2(II)	$1^3\Delta$ (66) +$1^1\Delta$ (28) +$1^3\Pi$ (6)	1.591	24530	8602	1655	24377	1557	6.714
0^- (II)	$1^3\Sigma^+$ (1)+$1^3\Pi$ (99)	1.603	24508	10642	1700	24382	1616	6.614
0^+ (III)	$A^1\Sigma^+$ (6)+$1^3\Pi$ (94)	1.598	24684	10466	1724	24573	1647	6.655
Exp. 0^+(III)	**$B^3\Pi_{0+}$**	**1.607**	**26420.9**	**9805**	**1670**	**26281.7**	**1567.3**	**6.582**
1(III)	$1^3\Delta$ (64) + $1^3\Pi$ (19) +$1^1\Pi$ (15) + $1^3\Sigma^+$ (2)	1.602	25633	9517	1614	25473	1549	6.622
Exp. 1(III)	**C1**	**1.610**	**27270.4**	**6912**	**1627**	**27101.3**	**1455.3**	**6.553**
1(IV)	$1^1\Pi$ (78) +$1^3\Delta$ (21) + $1^3\Sigma^+$ (1)	1.609	26495	8675	1659	26348	1569	6.564
Exp. 1(IV)	**c1**	**1.626**	**28161**	**8064**		**27957.5**	**1388.7**	**6.43**
2(III)	$1^1\Delta$ (70) +$1^3\Delta$ (22) +$1^3\Pi$ (8)	1.591	26684	8486	1654	26530	1551	6.714
Exp. 2(III)	**$b\Delta_2$**	**1.59**	**28470**	**7755**			**1475**	**6.7**
0^- (III)	$2^3\Sigma^+$ (100)	2.100	28260	4833	2041	28391	1591	3.854
1(V)	$2^3\Sigma^+$ (100)	2.088	28239	4855	2185	28259	1677	3.898

Table S2

Molecular states of CuH resulting from atomic states of Cu and H.

Atomic states	Molecular states
Cu (^{2}S) + H (^{2}S)	$^1\Sigma^+$, $^3\Sigma^+$
Cu (^{2}D) + H (^{2}S)	$^1\Sigma^+$, $^3\Sigma^+$, $^1\Pi$, $^3\Pi$, $^1\Delta$, $^3\Delta$
Cu (^{2}P^o) + H (^{2}S)	$^1\Sigma^+$, $^3\Sigma^+$, $^1\Pi$, $^3\Pi$
Cu (^{4}P^o) + H (^{2}S)	$^3\Sigma^+$, $^5\Sigma^+$, $^3\Pi$, $^5\Pi$
Cu (^{4}D^o) + H (^{2}S)	$^3\Sigma^-$, $^5\Sigma^-$, $^3\Pi$, $^5\Pi$, $^3\Delta$, $^5\Delta$
Cu (^{2}D^o) + H (^{2}S)	$^1\Sigma^-$ (2) , $^3\Sigma^-$ (2) , $^1\Pi$ (2) , $^3\Pi$ (2) , $^1\Delta$ (2) , $^3\Delta$ (2)
Cu (^{2}F^o) + H (^{2}S)	$^1\Sigma^+$ (2) , $^3\Sigma^+$ (2) , $^1\Pi$ (2) , $^3\Pi$ (2) , $^1\Delta$ (2) , $^3\Delta$ (2) , $^1\Phi$ (2) , $^3\Phi$ (2)
Cu (^{4}F^o) + H (^{2}S)	$^3\Sigma^+$, $^5\Sigma^+$, $^3\Pi$, $^5\Pi$, $^3\Delta$, $^5\Delta$, $^3\Phi$, $^5\Phi$

Table S3

Calculated spectroscopic constants (in cm^{-1}) for the ground and excited Ω states of CuH using an active space of 11 electrons in 10 orbitals. Experimental values are from references [8] and [17].

State (Ω)	Composition at r = 1.46 (Å)	r_e (Å)	T_e (cm^{-1})	D_e (cm^{-1})	ω_e (cm^{-1})	v_{0-0} (cm^{-1})	$\Delta G_{1/2}$ (cm^{-1})	B_e (cm^{-1})
0^+ (I)	$X^1\Sigma^+$ (100)	1.439	0	21870	1960	0	1875	8.207
Exp. 0^+(I)	**$X^1\Sigma^+$**	**1.463**	**0**	**22980**	**1941**	**0**	**1866.41**	**7.945**
0^- (I)	$1^3\Sigma^+$ (98)+ $1^3\Pi$ (2)	1.520	18297	3565	1794	18219	1711	7.356
1(I)	$1^3\Sigma^+$ (99) + $1^1\Pi$ (1)	1.519	18315	3548	1796	18238	1713	7.365
0^+ (II)	$A^1\Sigma^+$ (92)+ $1^3\Pi$ (8)	1.559	21592	9948	1706	21458	1608	6.992
Exp. 0^+(II)	**$A^1\Sigma^+$**	**1.572**	**23434.2**	**10748**	**1698**	**23311.1**	**1610.4**	**6.874**
2(I)	$1^3\Pi$ (87) +$1^3\Delta$ (12) +$1^1\Delta$ (1)	1.610	22649	8920	1649	22495	1548	6.556
1(II)	$1^3\Pi$ (80) +$1^1\Pi$ (6) +$1^3\Delta$ (14)	1.610	23033	8542	1650	22877	1543	6.556
3(I)	$1^3\Delta$ (100)	1.598	23449	8132	1608	23272	1498	6.655
2(II)	$1^3\Delta$ (69) +$1^1\Delta$ (25) +$1^3\Pi$ (6)	1.599	23929	7651	1607	23751	1493	6.647
0^- (II)	$1^3\Sigma^+$ (1)+$1^3\Pi$ (99)	1.608	23858	9754	1657	23711	1560	6.537
0^+ (III)	$A^1\Sigma^+$ (8)+$1^3\Pi$ (92)	1.604	24066	9530	1698	23933	1597	6.605
Exp. 0^+(III)	**$B^3\Pi_{0+}$**	**1.607**	**26420.9**	**9805**	**1670**	**26281.7**	**1567.3**	**6.582**
1(III)	$1^3\Delta$ (64) + $1^3\Pi$ (19) +$1^1\Pi$ (15) + $1^3\Sigma^+$ (2)	1.608	24996	8610	1595	24813	1480	6.573
Exp. 1(III)	**C1**	**1.610**	**27270.4**	**6912**	**1627**	**27101.3**	**1455.3**	**6.553**
1(IV)	$1^1\Pi$ (78) +$1^3\Delta$ (21) + $1^3\Sigma^+$ (1)	1.615	25860	7762	1600	25685	1498	6.516
Exp. 1(IV)	**c1**	**1.626**	**28161**	**8064**		**27957.5**	**1388.7**	**6.43**
2(III)	$1^1\Delta$ (73) +$1^3\Delta$ (20) +$1^3\Pi$ (7)	1.601	26147	7469	1596	25962	1476	6.630
Exp. 2(III)	**$b\Delta_2$**	**1.59**	**28470**	**7755**			**1475**	**6.7**
0^- (III)	$2^3\Sigma^+$ (100)	2.179	27140	4425	2137	27194	1556	3.579
1(V)	$2^3\Sigma^+$ (100)	2.187	27183	4377	2090	27255	1527	3.553

Table S4

MRCI potential energy curves (in cm^{-1}) for the ground and low-lying excited states of CuH using the largest active space that included the 3d, 3d′ and $4p_z$ orbitals of copper.

r (Å)	$X^1\Sigma^+$	$A^1\Sigma^+$	$1^3\Sigma^+$	$2^3\Sigma^+$	$1^1\Delta$	$1^3\Delta$	$1^1\Pi$	$1^3\Pi$
1.00	26982.09	58697.99	51895.59	95024.99	67121.29	66104.79	72152.33	69555.73
1.05	19407.28	49825.28	43475.68	83110.38	57572.78	56490.68	61691.66	59130.56
1.10	13570.84	42887.74	36901.74	73408.04	50028.54	48906.94	53343.32	50843.12
1.15	9152.51	37447.41	31803.91	65500.31	44084.01	42932.81	46726.75	44276.25
1.20	5882.34	33242.34	27897.84	59038.44	39434.34	38262.44	41523.34	39122.74
1.25	3519.67	30029.37	24950.57	53741.57	35846.17	34656.27	37462.40	35110.70
1.30	1877.45	27631.95	22790.15	49406.95	33117.55	31916.15	34340.32	32034.92
1.35	822.95	25890.65	21258.55	45848.65	31087.45	29869.75	31984.45	29727.95
1.40	232.52	24639.92	20232.62	42919.12	29620.12	28394.92	30243.41	28041.71
1.45	8.30	23900.40	19618.40	40499.80	28611.00	27386.20	29019.63	26860.93
1.46	0.00	23714.20	19536.60	40067.40	28455.30	27230.80	28824.82	26676.82
1.47	4.85	23719.25	19467.75	39653.35	28314.25	27088.45	28647.85	26509.65
1.50	79.86	23512.66	19331.36	38502.66	27976.46	26747.26	28199.03	26094.13
1.55	388.74	23387.54	19301.14	36854.84	27633.24	26406.94	27712.35	25654.55
1.60	870.69	23485.39	19467.29	35363.59	27525.99	26303.19	27492.76	25486.86
1.65	1493.76	23754.26	19782.46	34337.16	27604.76	26371.36	27482.78	25533.38
1.70	2217.41	24162.81	20206.21	33395.31	27823.71	26626.21	27634.18	25740.78
1.75	3007.64	24673.14	20702.74	32625.44	28151.14	26956.04	27916.77	26086.07
1.80	3869.62	25249.92	21250.72	32015.82	28562.72	27383.92	28283.46	26516.66
1.90	5677.37	26605.77	22371.37	31172.67	29515.77	28383.77	29201.01	27558.71
2.00	7520.41	27987.21	23296.81	30825.31	30510.21	29451.81	30223.32	28750.52
2.10	9327.20	29322.20	23776.10	30907.10	31457.30	30498.50	31212.16	29912.06
2.20	11048.76	30532.96	24010.46	31303.06	32286.76	31437.36	32095.89	30985.79
2.30	12655.81	31565.61	23945.91	31907.51	32956.21	32230.41	32832.96	31911.86
2.40	14123.99	32390.39	23749.99	32503.09	33458.09	32856.99	33408.04	32662.24
2.50	15439.56	33017.86	23581.56	33057.56	33815.96	33327.86	33818.67	33241.97
2.60	16600.54	33456.34	23477.24	33336.74	34054.24	33667.64	34102.40	33662.40
2.70	17603.07	33732.67	23230.37	33661.67	34218.57	33922.37	34289.41	33946.91
2.80	18460.91	33913.71	23103.61	33834.41	34306.41	34082.21	34405.76	34155.06
2.90	19192.26	34039.86	22952.56	33985.66	34353.46	34186.56	34477.79	34288.49
3.00	19803.93	34115.23	22838.43	34078.13	34374.63	34248.83	34514.04	34380.34
3.20	20735.81	34222.21	22664.51	34184.91	34409.61	34341.01	34548.96	34484.16
3.40	21331.10	34258.50	22546.50	34247.10	34418.30	34389.50	34544.57	34514.67
3.60	21698.25	34274.65	22466.05	34264.15	34408.15	34403.65	34540.52	34533.32
3.80	21933.87	34265.97	22411.37	34266.37	34399.37	34407.07	34533.86	34537.96
4.00	22077.60	34261.30	22379.00	34273.60	34391.60	34412.20	34531.10	34540.90
4.50	22242.33	34251.53	22341.53	34272.83	34385.13	34414.23	34523.40	34538.00
5.00	22293.39	34262.99	22335.89	34288.09	34395.99	34426.59	34528.96	34544.66
5.50	22305.86	34260.76	22334.36	34288.56	34394.26	34424.46	34528.34	34546.44
6.00	22310.89	34258.59	22331.89	34283.89	34390.99	34417.59	34528.31	34546.21
6.50	22309.29	34253.99	22328.79	34278.89	34389.79	34414.89	34529.55	34545.05
7.00	22305.02	34247.52	22323.52	34274.42	34381.52	34408.32	34523.89	34540.99
7.50	22307.63	34250.43	22327.33	34276.93	34383.63	34411.13	34523.89	34540.99
8.00	22308.24	34254.24	22327.64	34280.14	34386.74	34414.14	34529.24	34545.14
8.50	22308.28	34254.68	22327.88	34279.38	34386.78	34415.58	34529.02	34544.22
9.00	22308.50	34256.80	22327.70	34280.30	34388.30	34414.50	34529.29	34542.99

Table S5

Spin-orbit matrix elements (in cm^{-1}) for the ground and excited states of CuH.

r (Å)	$\langle 1^3\Delta \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Delta \rangle$	$\langle 1^3\Pi \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Pi \rangle$	$\langle 1^3\Sigma^+_{0-} \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Pi_{0-} \rangle$	$\langle 1^3\Sigma^+_{1} \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Pi_{1} \rangle$	$\langle 1^1\Delta \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Pi \rangle$	$\langle 1^3\Delta \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Pi \rangle$	$\langle 2^3\Sigma^+_{0-} \lvert \hat{\mathbf{H}}_{\mathbf{SO}} \rvert 1^3\Pi_{0-} \rangle$
1.00	-831.75	-414.07	-647.97	-456.82	-582.64	-587.57	-713.94
1.05	-830.12	-413.26	-689.70	-486.24	-582.21	-586.89	-676.95
1.10	-828.69	-412.64	-726.09	-511.89	-581.84	-586.29	-642.08
1.15	-827.47	-412.21	-757.66	-534.15	-581.46	-585.76	-609.53
1.20	-826.41	-411.94	-785.01	-553.43	-581.14	-585.31	-579.27
1.25	-825.47	-411.77	-808.44	-569.95	-580.85	-584.90	-551.59
1.30	-824.71	-411.68	-828.47	-584.07	-580.61	-584.58	-526.65
1.35	-823.99	-411.68	-845.70	-596.22	-580.45	-584.26	-503.89
1.40	-823.50	-411.69	-860.47	-606.63	-580.19	-584.00	-483.49
1.45	-823.05	-411.76	-873.09	-615.53	-579.99	-583.76	-465.17
1.46	-822.98	-411.79	-875.40	-617.16	-579.89	-583.70	-461.29
1.47	-822.90	-411.79	-877.60	-618.71	-579.91	-583.67	-458.43
1.50	-822.64	-411.85	-883.86	-623.12	-579.76	-583.53	-448.28
1.55	-822.33	-411.90	-893.05	-629.60	-579.60	-583.40	-434.50
1.60	-822.09	-411.95	-900.82	-635.08	-579.37	-582.95	-421.64
1.65	-821.87	-412.02	-907.28	-639.63	-579.18	-583.10	-411.04
1.70	-821.70	-412.06	-912.48	-643.30	-578.93	-582.69	-402.53
1.75	-821.44	-412.08	-916.73	-646.29	-578.86	-582.82	-395.30
1.80	-821.33	-412.07	-919.81	-648.47	-578.47	-582.70	-390.08
1.85	-821.19	-412.08	-921.75	-649.83	-578.25	-582.30	-387.25
1.90	-821.16	-412.04	-922.31	-650.23	-577.77	-582.31	-387.06
1.95	-821.04	-411.96	-921.40	-649.59	-577.32	-581.98	-389.57
2.00	-820.87	-411.91	-919.04	-647.93	-577.25	-581.89	-395.50
2.10	-820.72	-411.67	-904.41	-637.61	-576.97	-581.72	-429.95
2.20	-819.52	-410.20	-770.84	-543.44	-577.85	-580.38	-638.49
2.30	-818.54	-409.22	-490.93	-346.11	-577.21	-578.78	-870.95
2.40	-818.11	-408.87	-323.62	-228.15	-577.12	-578.78	-946.19
2.50	-817.86	-408.65	-215.08	-151.63	-577.49	-578.48	-976.73
2.60	-817.62	-408.50	-145.45	-102.54	-577.52	-578.26	-989.56
2.70	-817.49	-408.38	-100.74	-71.02	-577.52	-577.68	-995.18
2.80	-817.45	-408.27	-71.28	-50.25	-577.48	-578.63	-998.13
2.90	-817.37	-408.22	-51.21	-36.10	-577.47	-577.86	-999.06
3.00	-817.30	-408.21	-37.11	-26.16	-577.51	-577.80	-999.82
3.20	-817.25	-408.15	-20.40	-14.38	-577.50	-577.70	-1000.32
3.40	-817.22	-408.14	-11.40	-8.04	-577.53	-577.63	-1000.54
3.60	-817.22	-408.15	-6.64	-4.68	-577.56	-577.79	-1000.71
3.80	-817.22	-408.17	-3.91	-2.76	-577.58	-577.56	-1000.71
4.00	-817.21	-408.16	-2.39	-1.68	-577.58	-577.60	-1000.69
4.50	-817.19	-408.13	0.74	0.52	-577.56	-577.59	-1000.70
5.00	-817.19	-408.17	0.34	0.24	-577.61	-577.53	-1000.66
5.50	-817.20	-408.18	-0.23	-0.16	-575.85	-577.20	-1001.50
6.00	-817.21	-408.18	-0.14	-0.10	-573.01	-577.20	-1004.28
6.50	-817.22	-408.16	-0.14	-0.10	-577.85	-577.64	-1000.70
7.00	-817.23	-408.19	-0.10	-0.07	-576.88	-577.23	-1000.47
7.50	-817.22	-408.18	-0.13	-0.09	-579.76	-577.20	-1002.24
8.00	-817.22	-408.12	-0.15	-0.11	-577.99	-577.10	-1000.41
8.50	-817.22	-408.13	-0.15	-0.10	-581.86	-577.19	-1003.45
9.00	-817.21	-408.15	-0.07	-0.05	-582.47	-583.62	-997.19

Table S6

Spin-orbit matrix elements (in cm^{-1}) for the ground and excited states of CuH.

r (Å)	$\langle 2^3\Sigma_1^+ \lvert \hat{\mathbf{H}}_{SO} \rvert 1^3\Pi_1 \rangle$	$\langle X^1\Sigma^+ \lvert \hat{\mathbf{H}}_{SO} \rvert 1^3\Pi \rangle$	$\langle A^1\Sigma^+ \lvert \hat{\mathbf{H}}_{SO} \rvert 1^3\Pi \rangle$	$\langle 1^1\Delta \lvert \hat{\mathbf{H}}_{SO} \rvert 1^3\Delta \rangle$	$\langle 1^3\Sigma^+ \lvert \hat{\mathbf{H}}_{SO} \rvert 1^1\Pi \rangle$	$\langle 1^3\Delta \lvert \hat{\mathbf{H}}_{SO} \rvert 1^1\Pi \rangle$	$\langle 2^3\Sigma^+ \lvert \hat{\mathbf{H}}_{SO} \rvert 1^1\Pi \rangle$	$\langle 1^1\Pi \lvert \hat{\mathbf{H}}_{SO} \rvert 1^3\Pi \rangle$
1.00	-503.33	-428.08	-640.17	-831.04	-465.69	-592.46	-491.98	-410.56
1.05	-477.25	-446.11	-668.67	-829.28	-494.13	-591.05	-466.59	-409.79
1.10	-452.67	-459.32	-694.31	-827.73	-518.96	-589.14	-442.72	-409.21
1.15	-429.72	-468.38	-717.48	-826.38	-540.41	-588.62	-420.50	-408.82
1.20	-408.39	-474.23	-741.31	-825.16	-558.87	-587.61	-399.90	-408.58
1.25	-388.87	-476.86	-762.45	-824.08	-574.61	-586.67	-381.11	-408.43
1.30	-371.29	-477.03	-783.15	-823.16	-588.14	-585.88	-364.12	-408.37
1.35	-355.24	-474.86	-790.05	-822.33	-599.71	-585.15	-348.67	-408.38
1.40	-340.86	-471.09	-799.20	-821.64	-609.54	-584.49	-334.90	-408.43
1.45	-327.94	-466.20	-808.31	-821.02	-617.86	-583.92	-322.70	-408.52
1.46	-325.21	-464.88	-810.33	-820.92	-619.33	-583.83	-320.37	-408.52
1.47	-323.20	-463.86	-812.54	-820.81	-620.86	-583.24	-318.19	-408.56
1.50	-316.04	-460.01	-818.75	-820.49	-624.84	-583.43	-311.79	-408.60
1.55	-306.33	-452.99	-828.72	-819.96	-630.91	-583.00	-302.47	-408.71
1.60	-297.25	-444.29	-838.46	-819.48	-635.98	-582.61	-294.20	-408.78
1.65	-289.79	-435.18	-847.54	-819.06	-640.17	-582.27	-287.28	-408.88
1.70	-283.78	-425.27	-856.41	-818.64	-643.34	-581.98	-282.33	-408.94
1.75	-278.69	-414.74	-865.29	-818.59	-645.84	-581.68	-278.68	-408.99
1.80	-275.00	-403.66	-873.56	-817.86	-647.60	-581.46	-276.22	-408.98
1.85	-273.01	-392.18	-881.66	-817.50	-648.31	-580.71	-276.46	-408.92
1.90	-272.87	-381.38	-888.77	-817.93	-648.30	-581.01	-277.80	-408.86
1.95	-274.65	-370.17	-895.88	-817.04	-647.64	-580.78	-280.05	-408.83
2.00	-278.83	-360.78	-902.21	-817.39	-645.32	-579.88	-286.77	-408.64
2.10	-303.11	-357.90	-912.43	-816.43	-633.99	-579.85	-312.52	-408.64
2.20	-450.13	-325.13	-942.90	-817.57	-540.80	-578.85	-454.12	-408.57
2.30	-614.02	-269.79	-963.78	-817.30	-343.75	-578.05	-616.50	-408.11
2.40	-667.07	-233.47	-973.72	-817.13	-225.91	-577.78	-669.10	-408.02
2.50	-688.59	-202.08	-980.84	-817.06	-149.76	-577.65	-690.45	-407.99
2.60	-697.64	-173.69	-986.18	-816.97	-101.04	-577.56	-699.43	-407.97
2.70	-701.60	-148.02	-990.21	-816.96	-69.83	-577.10	-703.43	-407.97
2.80	-703.68	-125.02	-993.22	-817.02	-49.35	-576.84	-705.53	-407.94
2.90	-704.34	-104.34	-995.49	-817.02	-35.39	-577.47	-706.22	-407.95
3.00	-704.87	-86.01	-997.17	-817.02	-25.59	-577.51	-706.75	-408.01
3.20	-705.22	-56.51	-999.11	-817.07	-14.04	-577.11	-707.19	-408.01
3.40	-705.38	-35.66	-1000.03	-817.09	-7.81	-577.50	-707.37	-408.05
3.60	-705.50	-21.63	-1000.42	-817.13	-4.55	-577.16	-707.41	-408.10
3.80	-705.50	-12.76	-1000.58	-817.16	-2.68	-577.51	-707.56	-408.13
4.00	-705.49	-7.23	-1000.63	-817.16	-1.64	-577.57	-707.56	-408.14
4.50	-705.49	-1.50	-1000.67	-817.17	-0.50	-577.54	-707.59	-408.12
5.00	-705.47	-0.13	-1000.70	-817.18	-0.23	-577.67	-707.57	-408.16
5.50	-706.06	-0.12	-1001.69	-817.20	-0.14	-577.21	-708.18	-408.18
6.00	-708.02	-0.15	-1003.32	-817.21	-0.10	-577.20	-710.14	-408.18
6.50	-705.50	-0.12	-1000.82	-817.22	-0.12	-577.20	-707.58	-408.17
7.00	-705.33	-0.09	-1000.26	-817.22	-0.09	-577.21	-707.45	-408.18
7.50	-706.58	-0.11	-1001.93	-817.22	-0.10	-577.20	-706.49	-408.18
8.00	-705.29	-0.12	-1000.92	-817.22	-0.10	-577.10	-707.79	-408.12
8.50	-707.44	-0.12	-1003.15	-817.22	-0.07	-577.20	-709.55	-408.14
9.00	-703.02	-0.06	-997.86	-817.22	-0.07	-583.64	-705.13	-408.17

Table S7

SOC potential energy curves (in cm^{-1}) for the $\Omega = 0^+$ and 0^- states of CuH.

r (Å)	0^+(I)	0^+(II)	0^+(III)	0^-(I)	0^-(II)	0^-(III)
1.00	26985.81	58669.79	70018.19	51880.36	69980.62	95053.31
1.05	19410.31	49787.52	59602.54	43454.10	59561.95	83137.81
1.10	13573.22	42838.50	51326.58	36873.06	51281.81	73434.63
1.15	9154.32	37385.06	44772.91	31767.45	44723.01	65526.14
1.20	5883.64	33164.26	39635.41	27853.05	39578.25	59063.61
1.25	3520.54	29933.62	35641.26	24897.02	35575.25	53766.25
1.30	1877.99	27515.96	32586.05	22727.51	32508.89	49431.30
1.35	823.25	25756.95	30297.01	21186.63	30211.41	45872.78
1.40	232.64	24487.57	28629.60	20151.38	28534.49	42943.25
1.45	8.31	23725.10	27471.90	19527.93	27362.76	40524.12
1.46	0.00	23538.13	27288.62	19444.31	27180.44	40091.79
1.47	4.84	23533.37	27131.30	19373.66	27015.01	39677.83
1.50	79.82	23311.87	26730.75	19231.88	26604.61	38527.45
1.55	388.73	23160.53	26317.42	19193.05	26172.99	36880.34
1.60	870.78	23231.46	26176.68	19351.28	26011.98	35390.46
1.65	1493.99	23473.57	26249.79	19659.42	26064.17	34365.37
1.70	2217.83	23853.96	26485.24	20077.08	26275.47	33425.78
1.75	3008.29	24337.23	26857.31	20568.88	26622.25	32659.10
1.80	3870.53	24887.04	27314.63	21113.07	27052.12	32054.01
1.90	5678.81	26177.00	28421.96	22230.90	28079.64	31228.13
2.00	7522.37	27507.63	29664.00	23163.67	29216.54	30928.30
2.10	9329.07	28791.87	30876.17	23661.01	30200.41	31169.49
2.20	11051.53	29937.21	32012.89	23938.22	30756.80	32038.41
2.30	12660.07	30917.54	32988.86	23924.85	31239.69	33033.93
2.40	14129.08	31708.29	33772.09	23746.62	31811.81	33789.73
2.50	15445.29	32312.43	34374.22	23584.90	32343.20	34385.54
2.60	16606.79	32739.33	34805.62	23483.20	32657.23	34768.41
2.70	17609.74	33014.46	35090.75	23237.43	32962.92	35070.89
2.80	18467.92	33201.84	35292.12	23111.15	33144.71	35269.43
2.90	19199.53	33328.25	35424.95	22960.31	33288.81	35409.71
3.00	19811.42	33407.58	35512.65	22846.30	33380.32	35502.44
3.20	20743.57	33511.51	35619.18	22672.46	33485.56	35607.64
3.40	21338.99	33544.92	35652.51	22554.47	33536.89	35649.05
3.60	21706.19	33561.55	35670.57	22474.02	33554.42	35667.17
3.80	21941.84	33557.25	35670.84	22419.35	33557.43	35671.05
4.00	22085.57	33555.08	35671.24	22386.97	33563.17	35675.45
4.50	22250.31	33547.58	35666.08	22349.51	33561.65	35673.30
5.00	22301.37	33557.44	35674.33	22343.87	33574.01	35682.86
5.50	22313.84	33556.56	35674.79	22342.34	33574.91	35684.23
6.00	22318.87	33555.04	35673.89	22339.87	33571.76	35682.46
6.50	22317.27	33551.60	35671.59	22336.77	33568.08	35680.01
7.00	22313.00	33545.93	35666.69	22331.50	33563.75	35675.77
7.50	22315.61	33547.87	35667.72	22335.31	33565.42	35676.68
8.00	22316.22	33551.78	35671.73	22335.62	33568.93	35680.49
8.50	22316.26	33551.75	35671.24	22335.86	33568.09	35679.59
9.00	22316.48	33552.76	35671.12	22335.68	33568.30	35679.08

Table S8

SOC potential energy curves (in cm^{-1}) for the Ω = 1, 2, and 3 states of CuH.

r (Å)	1(I)	1(II)	1(III)	1(IV)	1(V)	2(I)	2(II)	2(III)	3(I)
1.00	51881.47	66736.94	69661.67	72271.09	95053.91	65630.62	67265.32	69495.97	65280.96
1.05	43455.78	57054.53	59296.79	61823.54	83138.45	56025.66	57524.95	59254.48	55668.54
1.10	36875.41	49367.10	51102.51	53491.45	73435.29	48440.43	49693.43	51256.48	48086.26
1.15	31770.63	43241.38	44675.08	46893.41	65526.84	42453.52	43395.06	45056.58	42113.33
1.20	27857.20	38374.31	39704.01	41711.20	59064.36	37749.81	38410.33	40271.82	37444.05
1.25	24902.25	34540.35	35902.35	37674.79	53767.05	34063.61	34558.27	36603.87	33838.80
1.30	22733.93	31571.88	33034.24	34580.98	49432.17	31173.20	31681.76	33826.37	31099.44
1.35	21194.33	29327.93	30901.28	32256.07	45873.74	28952.87	29581.85	31762.98	29053.68
1.40	20160.40	27682.34	29357.75	30550.40	42944.32	27313.67	28081.53	30273.99	27579.40
1.45	19538.32	26529.78	28290.63	29363.76	40525.36	26161.73	27057.72	29250.97	26571.13
1.46	19454.97	26349.85	28124.55	29176.85	40093.07	25981.85	26900.20	29093.15	26415.80
1.47	19384.59	26186.24	27972.74	29007.16	39679.14	25818.27	26756.54	28949.83	26273.53
1.50	19243.59	25780.59	27601.09	28582.89	38528.88	25412.81	26411.70	28605.62	25932.60
1.55	19206.07	25353.31	27215.41	28135.15	36882.07	24985.31	26065.41	28256.16	25592.64
1.60	19365.44	25191.97	27074.03	27951.70	35392.64	24824.79	25958.03	28145.31	25489.09
1.65	19674.54	25238.74	27118.42	27969.11	34368.08	24873.76	26028.29	28219.43	25557.47
1.70	20092.99	25448.90	27332.74	28160.23	33429.43	25085.74	26271.99	28445.02	25812.57
1.75	20585.27	25788.23	27648.85	28461.82	32664.26	25429.46	26602.25	28773.54	26142.49
1.80	21129.78	26213.69	28052.34	28854.11	32061.91	25859.67	27026.24	29189.47	26570.51
1.90	22247.35	27238.58	29010.02	29800.20	31252.28	26896.92	28015.73	30157.82	27570.66
2.00	23177.82	28392.62	29999.83	30743.87	31094.42	28074.28	29068.78	31182.10	28638.93
2.10	23671.61	29506.95	30651.40	31926.75	31409.95	29220.55	30090.74	32169.53	29685.74
2.20	23943.88	30479.34	31058.21	32846.71	32363.76	30275.48	30998.85	33049.52	30625.83
2.30	23926.54	31211.37	31637.32	33645.61	33266.31	31179.46	31754.88	33779.20	31419.85
2.40	23747.17	31831.65	32239.40	34262.99	33957.22	31904.67	32340.18	34347.89	32046.85
2.50	23585.09	32368.42	32719.52	34722.82	34489.50	32458.08	32771.09	34772.26	32518.02
2.60	23483.28	32690.24	33045.61	35032.97	34852.01	32855.04	33072.22	35072.92	32857.93
2.70	23237.46	32991.15	33284.57	35266.28	35128.66	33129.32	33285.31	35289.16	33112.80
2.80	23111.16	33169.47	33439.20	35409.61	35309.03	33316.13	33418.75	35424.89	33272.74
2.90	22960.32	33309.29	33539.73	35507.68	35431.23	33428.62	33506.34	35509.70	33377.17
3.00	22846.30	33396.45	33600.35	35565.80	35508.08	33489.08	33570.18	35560.64	33439.51
3.20	22672.46	33494.75	33671.86	35636.07	35605.49	33562.98	33655.95	35631.75	33531.74
3.40	22554.47	33541.60	33692.07	35662.20	35649.23	33594.22	33683.71	35660.43	33580.25
3.60	22474.02	33555.65	33700.59	35669.84	35664.75	33596.74	33698.23	35665.99	33594.41
3.80	22419.35	33556.74	33700.48	35669.92	35667.28	33594.02	33701.21	35664.98	33597.84
4.00	22386.97	33561.47	33701.69	35673.79	35669.96	33592.48	33703.39	35664.64	33602.96
4.50	22349.51	33559.07	33698.11	35673.50	35666.96	33590.01	33700.94	35662.31	33605.02
5.00	22343.87	33571.18	33705.63	35684.28	35676.38	33601.54	33708.79	35672.82	33617.38
5.50	22342.34	33571.64	33705.58	35683.71	35676.18	33599.62	33709.65	35671.75	33615.24
6.00	22339.87	33568.54	33703.93	35679.91	35673.10	33594.67	33708.18	35667.74	33608.36
6.50	22336.77	33565.32	33703.38	35677.44	35671.47	33592.75	33706.86	35665.99	33605.64
7.00	22331.50	33560.68	33698.21	35672.47	35665.53	33585.29	33702.12	35659.33	33599.07
7.50	22335.31	33562.34	33698.78	35673.82	35667.24	33587.73	33702.65	35661.23	33601.89
8.00	22335.62	33566.08	33703.10	35677.50	35671.16	33590.79	33706.53	35664.53	33604.90
8.50	22335.86	33565.40	33702.95	35677.68	35671.90	33591.49	33706.00	35664.89	33606.34
9.00	22335.68	33565.87	33702.41	35676.96	35671.61	33591.79	33705.10	35664.79	33605.26

Table S9

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the $\Omega = 0^+$ states of CuH.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp. [8,17]**	Matrix Eigenvectors
0^+(I) v = 0	0	0	**0**	$X^1\Sigma^+$ (1 v=0)
0^+(I) v = 1	1866	1866	**1866.41**	$X^1\Sigma^+$ (1 v=1)
0^+(I) v = 2	3654	3655	**3658.47**	$X^1\Sigma^+$ (1 v=2)
0^+(I) v = 3	5371	5373	**5376.85**	$X^1\Sigma^+$ (1 v=3)
0^+(I) v = 4	7013	7016	**7021.93**	$X^1\Sigma^+$ (1 v=4)
0^+(I) v = 5	8582	8584		$X^1\Sigma^+$ (1 v=5)
0^+(I) v = 6	10077	10080		$X^1\Sigma^+$ (1 v=6)
0^+(I) v = 7	11500	11503		$X^1\Sigma^+$ (1 v=7)
0^+(I) v = 8	12847	12851		$X^1\Sigma^+$ (1 v=8)
0^+(I) v = 9	14118	14122		$X^1\Sigma^+$ (1 v=9)
0^+(I) v =10	15308	15311		$X^1\Sigma^+$ (1 v=10)
0^+(II) v = 0	23039	23043	**23311**	$A^1\Sigma^+$ (0.95 v=0) + $1^3\Pi$ (0.5 v=0)
0^+(II) v = 1	24667	24663	**24922**	$A^1\Sigma^+$ (0.94 v=1) + $1^3\Pi$ (0.3 v=1) + $1^3\Pi$ (0.3 v=0)
0^+(II) v = 2	26205	26196	**26444**	$A^1\Sigma^+$ (0.92 v=2) + $1^3\Pi$ (0.3 v=1) + $1^3\Pi$ (0.3 v=2) + $A^1\Sigma^+$ (0.1 v=1) + $A^1\Sigma^+$ (0.1 v=3)
0^+(II) v = 3	27646	27648	**27877**	$1^3\Pi$ (-0.60 v=1) + $A^1\Sigma^+$ (-0.70 v=3) + $A^1\Sigma^+$ (0.20 v=1) + $1^3\Pi$ (0.30 v=2) + $1^3\Pi$ (0.20 v=3)
0^+(II) v = 4	28976	28965	**29176**	$A^1\Sigma^+$ (-0.90 v=4) + $A^1\Sigma^+$ (-0.20 v=3) + $1^3\Pi$ (-0.20 v=4) + $1^3\Pi$ (-0.40 v=3)
0^+(II) v = 5	30180	30178	**30358**	$A^1\Sigma^+$ (0.16 v=4) + $A^1\Sigma^+$ (0.86 v=5) + $1^3\Pi$ (-0.4 v=4) + $1^3\Pi$ (-0.20 v=5)
0^+(II) v = 6	31223	31243	**31378**	$A^1\Sigma^+$ (-0.83 v=6) + $A^1\Sigma^+$ (-0.18 v=5) + $1^3\Pi$ (-0.21 v=6) +$1^3\Pi$ (-0.44 v=5)
0^+(II) v = 7	32047	32094		$A^1\Sigma^+$ (0.20 v=6) + $A^1\Sigma^+$ (0.78 v=7) + $A^1\Sigma^+$ (-0.24 v=8) + $1^3\Pi$ (-0.47 v=6) + $1^3\Pi$ (-0.23 v=7)
0^+(II) v = 8	32534	32636		$A^1\Sigma^+$ (-0.14 v=6) + $A^1\Sigma^+$ (-0.28 v=7) + $A^1\Sigma^+$ (-0.79 v=8) + $1^3\Pi$ (0.10 v=6) + $1^3\Pi$ (-0.50 v=7)
0^+(III) v = 0	26035	26043	**26282**	$A^1\Sigma^+$ (-0.3 v=0) + $A^1\Sigma^+$ (0.3 v=1) + $1^3\Pi$ (0.94 v=0)
0^+(III) v = 1	27617	27618	**27844**	$1^3\Pi$ (0.70 v=1) +$A^1\Sigma^+$ (-0.60 v=3) + $A^1\Sigma^+$ (-0.30 v=2) + $A^1\Sigma^+$ (0.20 v=1) + $1^3\Pi$ (0.20 v=2) + $1^3\Pi$ (0.10 v=3)
0^+(III) v = 2	29106	29125	**29328**	$A^1\Sigma^+$ (0.20 v=2) + $A^1\Sigma^+$ (-0.30 v=3) + $1^3\Pi$ (-0.90 v=2) + $1^3\Pi$ (0.14 v=3)
0^+(III) v = 3	30492	30512		$A^1\Sigma^+$ (0.35 v=4) + $A^1\Sigma^+$ (-0.23 v=3) + $1^3\Pi$ (0.14 v=4) + $1^3\Pi$ (-0.90 v=3)
0^+(III) v = 4	31758	31777		$A^1\Sigma^+$ (0.2 v=4) + $A^1\Sigma^+$ (-0.4 v=5) + $1^3\Pi$ (-0.86 v=4) + $1^3\Pi$ (0.15 v=5)

Table S10

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the $\Omega = 0^-$ states of CuH.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp.**	Matrix Eigenvectors
0^-(I) v = 0	19055	19056		$1^3\Sigma^+$ (0.99 v=0) + $1^3\Pi$ (-0.12 v=0)
0^-(I) v = 1	20647	20647		$1^3\Sigma^+$ (0.99 v=1)
0^-(I) v = 2	22071	22072		$1^3\Sigma^+$ (0.99 v=2) + $1^3\Pi$ (0.10 v=2)
0^-(II) v = 0	25851	25864		$1^3\Pi$ (0.99 v=0)
0^-(II) v = 1	27394	27404		$1^3\Sigma^+$ (0.10 v=1) + $1^3\Pi$ (-0.98 v=1)
0^-(II) v = 2	28813	28792		$2^3\Sigma^+$ (0.16 v=0) + $1^3\Pi$ (0.97 v=2)
0^-(II) v = 3	30013	29935		$2^3\Sigma^+$ (0.46 v=0) + $2^3\Sigma^+$(0.14 v=1) + $1^3\Pi$ (0.85 v=3) + $1^3\Pi$ (0.12 v=4)
0^-(III) v = 0	30641	30540		$2^3\Sigma^+$ (0.80 v=0) + $1^3\Pi$ (-0.10 v=2) + $1^3\Pi$ (-0.50 v=3) + $1^3\Pi$ (0.27 v=4)
0^-(III) v = 1	31967	31980		$2^3\Sigma^+$ (0.43 v=1) + $2^3\Sigma^+$ (0.35 v=2) + $2^3\Sigma^+$ (0.10 v=3) + $1^3\Pi$ (-0.66 v=4) + $1^3\Pi$ (0.45 v=5) + $1^3\Pi$ (0.19 v=6)

Table S11

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the Ω = 1 states of CuH.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp. [8]**	Matrix Eigenvectors
1(I) v = 0	19068	19068		$1^3\Sigma^+$ (1 v=0)
1(I) v = 1	20660	20660		$1^3\Sigma^+$ (1 v=1)
1(I) v = 2	22085	22085		$1^3\Sigma^+$ (1 v=2)
1(II) v = 0	25024	25169		$1^1\Pi$ (-0.14 v=0) + $1^3\Pi$ (-0.95 v=0) + $1^3\Delta$ (0.27 v=0)
1(II) v = 1	26560	26552		$1^3\Pi$ (0.14 v=1) + $1^1\Pi$ (0.63 v=0) + $1^3\Pi$ (0.12 v=0) + $1^3\Delta$ (0.75 v=0)
1(II) v = 2	27994	28089		$1^3\Pi$ (0.13 v=0) + $1^1\Pi$ (-0.35 v=0) + $1^3\Pi$ (0.37 v=2) + $1^3\Delta$ (0.28 v=0) +$1^1\Pi$ (0.52 v=1) + $1^3\Delta$ (0.60 v=1)
1(II) v = 3	29307	29429		$2^3\Sigma^+$ (-0.17 v=0) + $1^3\Pi$ (0.93 v=3) + $1^3\Delta$ (-0.29 v=3)
1(III) v = 0	26881	26716	**27101**	$1^1\Pi$ (0.14 v=1) + $1^3\Pi$ (0.94 v=1) + $1^3\Delta$ (-0.11 v=0) + $1^3\Delta$ (-0.27 v=1)
1(III) v = 1	28357	28151	**28557**	$1^1\Pi$ (-0.23 v=1) + $1^1\Pi$ (0.12 v=2) + $1^3\Pi$ (0.87 v=2) + $1^3\Delta$ (-0.27 v=1) +$1^3\Delta$(-0.27 v=2)
1(III) v = 2	29659	29540	**29840**	$1^1\Pi$ (-0.50 v=1) + $1^1\Pi$ (0.50 v=2) + $1^3\Pi$ (0.19 v=1) + $1^3\Delta$ (0.40 v=1) +$1^3\Delta$ (0.54 v=2)
1(III) v = 3	30649	30918		$2^3\Sigma^+$ (0.30 v=0) + $1^1\Pi$ (-0.60 v=2) + $1^1\Pi$ (0.32 v=3) +$1^1\Pi$ (0.11 v=4) + $1^3\Pi$ (0.24 v=2) + $1^3\Pi$ (0.30 v=4) + $1^3\Delta$ (0.48 v=2) + $1^3\Delta$ (0.18 v=3)
1(IV) v = 0	27757	27890	**27958**	$1^1\Pi$ (-0.66 v=0) + $1^1\Pi$ (-0.31 v=1) + $1^3\Pi$ (0.23 v=0) +$1^3\Delta$ (0.52 v=0) + $1^3\Delta$ (-0.36 v=1)
1(IV) v = 1	29244	29280	**29346**	$2^3\Sigma^+$(-0.14 v=0) + $1^1\Pi$ (-0.54 v=1) + $1^1\Pi$ (-0.45 v=2) + $1^3\Pi$ (0.19 v=1) + $1^3\Delta$ (0.45 v=1) + $1^3\Delta$ (-0.48 v=2)
1(IV) v = 2	30610	30563	**30940**	$2^3\Sigma^+$ (-0.19 v=1) + $1^1\Pi$ (0.31 v=2) + $1^1\Pi$ (0.28 v=3) +$1^3\Pi$ (-0.11 v=2) + $1^3\Pi$ (0.73 v=4) + $1^3\Delta$ (-0.25 v=2) + $1^3\Delta$ (0.32 v=3) +$1^3\Delta$ (-0.23 v=4)
1(IV) v = 3	31887	31878		$2^3\Sigma^+$ (-0.50 v=1) + $2^3\Sigma^+$ (0.39 v=2) + $1^1\Pi$ (0.42 v=4) + $1^3\Pi$ (-0.16 v=5) +$1^3\Pi$ (-0.16 v=6) + $1^3\Delta$ (0.57 v=4) + $1^3\Delta$ (0.15 v=5)
1(V) v = 0	30787	30728		$2^3\Sigma^+$ (0.48 v=0) + $2^3\Sigma^+$ (-0.22 v=1) + $1^1\Pi$ (-0.45 v=3) +$1^3\Pi$ (0.37 v=4) + $1^3\Delta$ (-0.57 v=3) + $1^3\Delta$ (-0.16 v=4)
1(V) v = 1	32119	32143		$2^3\Sigma^+$ (-0.20 v=1) + $2^3\Sigma^+$ (0.24 v=2) + $2^3\Sigma^+$ (0.22 v=3) + $1^1\Pi$ (0.57 v=3) + $1^1\Pi$ (-0.30 v=4) + $1^3\Pi$ (-0.24 v=3) + $1^3\Pi$ (-0.29 v=6) + $1^3\Pi$ (-0.12 v=7) + $1^3\Delta$ (-0.48 v=3) + $1^3\Delta$ (-0.15 v=4) + $1^3\Delta$ (0.12 v=6)
1(V) v = 2	33261	33193		$2^3\Sigma^+$ (-0.15 v=1) + $2^3\Sigma^+$ (-0.11 v=2) + $1^1\Pi$ (0.60 v=4) + $1^1\Pi$ (-0.33 v=5) + $1^3\Pi$ (-0.29 v=4) +$1^3\Pi$ (-0.12 v=6) +$1^3\Pi$ (-0.24 v=7) + $1^3\Delta$ (-0.57 v=4)

Table S12

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the Ω = 2 and 3 states of CuH.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp. [8]**	Matrix Eigenvectors
2(I) v = 0	24660	24660		$1^1\Delta$ (0.11 v=0) + $1^3\Delta$ (0.31 v=0) + $1^3\Pi$ (-0.94 v=0)
2(I) v = 1	26204	26209		$1^1\Delta$ (-0.11 v=1) + $1^3\Delta$ (0.32 v=1) + $1^3\Pi$ (-0.94 v=1)
2(I) v = 2	27649	27657		$1^1\Delta$ (0.11 v=2) + $1^3\Delta$ (0.33 v=2) + $1^3\Pi$ (-0.93 v=2)
2(I) v = 3	28986	28994		$1^1\Delta$ (0.10 v=3) + $1^3\Delta$ (0.35 v=3) + $1^3\Pi$ (0.93 v=3)
2(I) v = 4	30190	30200		$1^3\Delta$ (0.37 v=4) + $1^3\Pi$ (-0.92 v=4)
2(II) v = 0	25774	25769		$1^1\Delta$ (0.52 v=0) + $1^3\Delta$ (0.83 v=0) +$1^3\Pi$ (0.22 v=0)
2(II) v = 1	27269	27262		$1^1\Delta$ (0.57 v=1) + $1^3\Delta$ (0.82 v=1) + $1^3\Pi$ (0.22 v=1)
2(II) v = 2	28652	28646		$1^1\Delta$ (0.53 v=2) + $1^3\Delta$ (0.81 v=2) + $1^3\Pi$ (0.23 v=2)
2(II) v = 3	29908	29902		$1^1\Delta$ (0.54 v=3) + $1^1\Delta$ (0.80 v=3) + $1^3\Pi$ (0.24 v=3)
2(II) v = 4	31012	30994		$1^1\Delta$ (0.55 v=4) + $1^3\Delta$ (0.75 v=4) + $1^3\Pi$ (0.24 v=4)
2(III) v = 0	27957	27956		$1^1\Delta$ (0.85 v=0) + $1^3\Delta$ (0.46 v=0) +$1^3\Pi$ (-0.25 v=0)
2(III) v = 1	29439	29436	**29725**	$1^1\Delta$ (0.85 v=1) + $1^3\Delta$0.46 v=1) + $1^3\Pi$ (0.26 v=1)
2(III) v = 2	30804	30798		$1^1\Delta$ (0.83 v=2) + $1^3\Delta$ (0.47 v=2) + $1^3\Pi$ (0.26 v=2)
2(III) v = 3	32036	32033		$1^1\Delta$ (0.82 v=3) + $1^3\Delta$ (0.47 v=3) + $1^3\Pi$ (0.27 v=3)
2(III) v = 4	33111	33107		$1^1\Delta$ (0.80 v=4) + $1^3\Delta$ (0.49 v=4) + $1^3\Delta$ (0.13 v=5) + $1^3\Pi$ (-0.29 v=4)
3(I) v = 0	25305	25305		$1^3\Delta$ (1 v=0)
3(I) v = 1	26804	26804		$1^3\Delta$ (1 v=1)
3(I) v = 2	28193	28193		$1^3\Delta$ (1 v=2)
3(I) v = 3	29463	29463		$1^3\Delta$ (1 v=3)
3(I) v = 4	30593	30593		$1^3\Delta$ (1 v=4)
3(I) v = 5	31542	31542		$1^3\Delta$ (1 v=5)
3(I) v = 6	32251	32251		$1^3\Delta$ (1 v=6)
3(I) v = 7	32616	32616		$1^3\Delta$ (1 v=7)

Table S13

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the $\Omega = 0^+$ states of CuD.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp. [8,17]**	Matrix Eigenvectors
0^+(I) v = 0	0	0	**0**	$X^1\Sigma^+$ (1 v=0)
0^+(I) v = 1	1347	1347	**1346.22**	$X^1\Sigma^+$ (1 v=1)
0^+(I) v = 2	2652	2653	**2654.45**	$X^1\Sigma^+$ (1 v=2)
0^+(I) v = 3	3920	3921	**3925.00**	$X^1\Sigma^+$ (1 v=3)
0^+(I) v = 4	5152	5154	**5158.07**	$X^1\Sigma^+$ (1 v=4)
0^+(I) v = 5	6346	6348		$X^1\Sigma^+$ (1 v=5)
0^+(I) v = 6	7502	7504		$X^1\Sigma^+$ (1 v=6)
0^+(I) v = 7	8621	8623		$X^1\Sigma^+$ (1 v=7)
0^+(I) v = 8	9703	9705		$X^1\Sigma^+$ (1 v=8)
0^+(I) v = 9	10747	10750		$X^1\Sigma^+$ (1 v=9)
0^+(I) v = 10	11755	11758		$X^1\Sigma^+$ (1 v=10)
0^+(II) v = 0	23073	23075	**23326**	$A^1\Sigma^+$ (0.98 v=0) + $1^3\Pi$ (-0.2 v=0)
0^+(II) v = 1	24254	24253	**24497**	$A^1\Sigma^+$ (-0.95 v=1) + $1^3\Pi$ (0.26 v=1) +$1^3\Pi$ (0.16 v=0)
0^+(II) v = 0	25384	25383	**25622**	$A^1\Sigma^+$ 0.94 v=2) +$1^3\Pi$ (0.22 v=1) + $1^3\Pi$ (0.23 v=2)
0^+(II) v = 1	26470	26466	**26700**	$A^1\Sigma^+$ (0.92 v=3) +$1^3\Pi$ (-0.27 v=2) + $1^3\Pi$ (-0.20 v=3)
0^+(II) v = 2	27510	27505	**27728**	$A^1\Sigma^+$ (-0.13 v=3) + $A^1\Sigma^+$ (-0.91 v=4) + $1^3\Pi$ (-0.30 v=3) +$1^3\Pi$ (-0.18 v=4) + $1^3\Pi$ (0.10 v=5)
0^+(II) v = 3	28498	28494	**28701**	$A^1\Sigma^+$ (-0.15 v=4) + $A^1\Sigma^+$ (-0.90 v=5) + $1^3\Pi$ (0.34 v=4) +$1^3\Pi$ (0.16 v=5)
0^+(II) v = 4	29426	29429	**29617**	$A^1\Sigma^+$ (0.19 v=5) + $A^1\Sigma^+$ (0.84 v=6) + $A^1\Sigma^+$ (-0.11 v=7) + $1^3\Pi$ (0.36 v=5) + $1^3\Pi$ (0.13 v=6)
0^+(II) v = 5	30283	30288		$A^1\Sigma^+$ (0.17 v=6) + $A^1\Sigma^+$ (-0.84 v=7) + $A^1\Sigma^+$ (0.14 v=8) +$1^3\Pi$ (-0.17 v=4) +$1^3\Pi$ (0.16 v=5) +$1^3\Pi$ (0.39 v=6) + $1^3\Pi$ (0.12 v=7)
0^+(III) v = 0	26075	26079	**26297**	$A^1\Sigma^+$ (-0.27 v=0) + $A^1\Sigma^+$ (0.15 v=1) +$1^3\Pi$ (0.94 v=0)
0^+(III) v = 1	27222	27228	**27449**	$A^1\Sigma^+$ (0.25 v=1) + $A^1\Sigma^+$ (-0.22 v=2) + $1^3\Pi$ (0.93 v=1)
0^+(III) v = 2	28322	28329	**28527**	$A^1\Sigma^+$ (0.23 v=2) + $A^1\Sigma^+$ (-0.26 v=3) + $1^3\Pi$ (-0.92 v=2) + $1^3\Pi$ (0.12 v=3)
0^+(III) v = 3	29376	29380		$A^1\Sigma^+$ (-0.19 v=3) + $A^1\Sigma^+$ (0.30 v=4) + $1^3\Pi$ (-0.87 v=3) + $1^3\Pi$ (0.17 v=4)

Table S14

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the $\Omega = 0^-$ states of CuD.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp.**	Matrix Eigenvectors
0^-(I) v = 0	19092	19093		$1^3\Sigma^+$ (-0.99 v=0) + $1^3\Pi$ (-0.11 v=0)
0^-(I) v = 1	20254	20254		$1^3\Sigma^+$ 1 v=1)
0^-(I) v = 2	21349	21350		$1^3\Sigma^+$ (1 v=2)
0^-(II) v = 0	25896	25909		$1^3\Pi$ (1 v=0)
0^-(II) v = 1	27019	27026		$1^3\Pi$ (1 v=1)
0^-(II) v = 2	28085	28031		$1^3\Pi$ (1 v=2)
0^-(II) v = 3	29088	29005		$2^3\Sigma^+$ (0.15 v=0) + $1^3\Pi$ (0.98 v=3)
0^-(II) v = 4	29975	29894		$2^3\Sigma^+$ (-0.34 v=0) + $2^3\Sigma^+$ (-0.13 v=1) + $1^3\Pi$ (-0.92 v=4) + $1^3\Pi$ (-0.11 v=5)
0^-(III) v = 0	30722	30843		$2^3\Sigma^+$ (0.62 v=0) + $2^3\Sigma^+$ (-0.49 v=1) +$1^3\Pi$ (-0.57 v=5) + $1^3\Pi$ (-0.12 v=6)
0^-(III) v = 1	31692	31700		$2^3\Sigma^+$ (0.49 v=1) + $2^3\Sigma^+$ (0.34 v=2) + $1^3\Pi$ (-0.55 v=5) + $1^3\Pi$ (0.51 v=6) + $1^3\Pi$ (0.23 v=7)

Table S15

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the Ω = 1 states of CuD.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp. [8]**	Matrix Eigenvectors
1(I) v = 0	19105	19105		$1^3\Sigma^+$ (1 v=0)
1(I) v = 1	20267	20266		$1^3\Sigma^+$ (1 v=1)
1(I) v = 2	21363	21363		$1^3\Sigma^+$ (1 v=2)
1(II) v = 0	25071	25214		$1^1\Pi$ (-0.14 v=0) + $1^3\Pi$ (-0.95 v=0) +$1^3\Delta$ (0.27 v=0)
1(II) v = 1	26187	26332		$1^1\Pi$ (0.13 v=1) + $1^3\Pi$ (0.94 v=1) +$1^3\Delta$ (-0.27 v=1)
1(II) v = 2	27251	27378		$1^1\Pi$ (-0.11 v=2) + $1^3\Pi$ (-0.95 v=2) +$1^3\Delta$ (0.27 v=2)
1(II) v = 3	28265	28385		$1^1\Pi$ (-0.26 v=3) + $1^3\Pi$ (-0.88 v=3) + $1^3\Delta$ (-0.35 v=3)
1(II) v = 4	29216	29335		$1^1\Pi$ (0.10 v=3) + $1^3\Pi$ (0.95 v=3) + $1^3\Delta$ (-0.28 v=3)
1(II) v = 5	30088	30100		$2^3\Sigma^+$ (0.23 v=0) +$1^1\Pi$ (0.27 v=3) + $1^3\Pi$ (-0.23 v=2) + $1^3\Pi$ (-0.12 v=5) +$1^3\Delta$ (-0.52 v=2) + $1^3\Delta$ (-0.36 v=3)
1(III) v = 0	26936	26613	**27149**	$1^1\Pi$ (0.63 v=0) + $1^3\Pi$ (0.12 v=0) +$1^3\Delta$ (0.75 v=0)
1(III) v = 1	28014	28023	**28232**	$1^1\Pi$ (-0.72 v=0) +$1^1\Pi$ (0.19 v=1) + $1^3\Pi$ (0.26 v=0) + $1^3\Delta$ (0.57 v=0) + $1^3\Delta$ (0.6923 v=1)
1(III) v = 2	29028	29108	**29256**	$1^1\Pi$ (0.69 v=1) + $1^1\Pi$ (-0.24 v=2) + $1^3\Pi$ (-0.25 v=1) + $1^3\Delta$ (-0.55 v=1) + $1^3\Delta$ (-0.27 v=2)
1(III) v = 3	29934	30191		$2^3\Sigma^+$ (0.27 v=0) + $1^1\Pi$ (0.21 v=2) +$1^1\Pi$ (-0.15 v=3) + $1^3\Pi$ (-0.86 v=5) + $1^3\Delta$ (0.28 v=5)
1(IV) v = 0	27810	27673	**27989**	$1^1\Pi$ (-0.23 v=0) + $1^1\Pi$ (-0.61 v=1) + $1^3\Pi$ (-0.12 v=0) + $1^3\Delta$ (-0.18 v=0) + $1^3\Delta$ (-0.71 v=1)
1(IV) v = 1	28895	28675		$1^1\Pi$ (0.27 v=1) + $1^1\Pi$ (0.61 v=2) + $1^3\Pi$ (0.13 v=2) + $1^3\Delta$ (-0.23 v=1) + $1^3\Delta$ (0.68 v=2)
1(IV) v = 2	29914	29613	**30230**	$2^3\Sigma^+$ (0.17 v=0) + $1^1\Pi$ (0.61 v=3) + $1^1\Pi$ (-0.22 v=3) + $1^3\Pi$ (0.13 v=3+ $1^3\Delta$ (-0.28 v=2) + $1^3\Delta$ (0.62 v=3)
1(IV) v = 3	30876	30914		$2^3\Sigma^+$ (-0.13 v=0) + $2^3\Sigma^+$ (0.51 v=1) + $2^3\Sigma^+$ (0.24 v=2) + $1^1\Pi$ (-0.19 v=3) + $1^1\Pi$ (0.17 v=5) + $1^3\Pi$ (0.14 v=5) + $1^3\Pi$ (-0.67 v=6) + $1^3\Pi$ (-0.15 v=7) + $1^3\Delta$ (0.17 v=3) + $1^3\Delta$ (0.25 v=6)
1(V) v = 0	30867	30701		$2^3\Sigma^+$ (0.64 v=0) + $1^1\Pi$ (-0.19 v=2) + $1^1\Pi$ (-0.38 v=4) + $1^1\Pi$ (0.14 v=5) + $1^3\Pi$ (0.18 v=5) + $1^3\Delta$ (-0.58 v=4)
1(V) v = 1	31841	31607		$2^3\Sigma^+$ (0.49 v=1) + $2^3\Sigma^+$ (-0.54 v=2) + $2^3\Sigma^+$ (0.20 v=3) + $1^1\Pi$ (0.18 v=5) + $1^3\Pi$ (0.44 v=7) + $1^3\Pi$ (0.16 v=8) + $1^3\Delta$ (-0.32 v=5)
1(V) v = 2	32759	32591		$2^3\Sigma^+$ (0.15 v=2) + $2^3\Sigma^+$ (-0.33 v=3) + $2^3\Sigma^+$ (0.29 v=2) + $1^1\Pi$ (0.23 v=5) + $1^1\Pi$ (-0.34 v=6+ $1^1\Pi$ (-0.43 v=7) +$1^1\Pi$ (0.12 v=8) + $1^3\Pi$ (-0.43 v=8) + $1^3\Pi$ (-0.13 v=10) + $1^3\Delta$ (-0.27 v=5) + $1^3\Delta$ (-0.29 v=7) + $1^3\Delta$ (0.11 v=8)
1(V) v = 3	33526	33618		$2^3\Sigma^+$ (0.15 v=2) + $2^3\Sigma^+$ (0.10 v=5) + $1^1\Pi$ (-0.11 v=5) + $1^1\Pi$ (-0.52 v=6) + $1^1\Pi$ (0.27 v=7) + $1^1\Pi$ (-0.35 v=8) + $1^3\Pi$ (0.26 v=6) ++ $1^3\Pi$ (-0.28 v=10) + $1^3\Delta$ (0.52 v=6) + $1^3\Delta$ (-0.12 v=8) + $1^3\Delta$ (-0.13 v=9)

Table S16

Vibronic energies (in cm^{-1}) obtained from the SOC-corrected potential energy curves (E_{SOC}) and the eigenvalues (E_{Matrix}) and eigenvectors from diagonalization of the SOC matrix for the Ω = 2 and 3 states of CuD.

State (Ω)	E_{SOC}	E_{Matrix}	**Exp.**	Matrix Eigenvectors
2(I) v = 0	24706	24706		$1^1\Delta$ (0.11 v=0) + $1^3\Delta$ (-0.31 v=0) + $1^3\Pi$ (0.95 v=0)
2(I) v = 1	25827	25811		$1^1\Delta$ (0.36 v=0) + $1^3\Delta$ (0.61 v=0) + $1^3\Delta$ (-0.21 v=1) + $1^3\Pi$ (0.16 v=0) + $1^3\Pi$ (0.64 v=1)
2(I) v = 2	26896	26885		$1^1\Delta$ (0.28 v=1) + $1^3\Delta$ (0.49 v=1) + $1^3\Delta$ (-0.26 v=2) + $1^3\Pi$ (0.13 v=1) + $1^3\Pi$ (0.76 v=2)
2(I) v = 3	27919	27911		$1^1\Delta$ (0.25 v=2) + $1^3\Delta$ (0.43 v=2) + $1^3\Delta$ (0.29 v=3) + $1^3\Pi$ (0.12 v=2) + $1^3\Pi$ (0.80 v=3)
2(I) v = 4	28884	28882		$1^1\Delta$ (0.21 v=3) + $1^3\Delta$ (0.34 v=3) + $1^3\Delta$ (0.31 v=4) + $1^3\Pi$ (0.85 v=4)
2(II) v = 0	25827	25842		$1^1\Delta$ (0.36 v=0) + $1^3\Delta$ (-0.56 v=0) + $1^3\Delta$ (-0.23 v=1) + $1^3\Pi$ (-0.14 v=0) + $1^3\Pi$ (0.69 v=1)
2(II) v = 1	26914	26926		$1^1\Delta$ (0.43 v=1) + $1^3\Delta$ (-0.67 v=1) + $1^3\Delta$ (-0.19 v=2) + $1^3\Pi$ (-0.18 v=1) + $1^3\Pi$ (0.55 v=2)
2(II) v = 2	27947	27953		$1^1\Delta$ (-0.12 v=0) + $1^1\Delta$ (0.45 v=2) + $1^3\Delta$ (-0.70 v=2) + $1^3\Delta$ (-0.17 v=3) + $1^3\Pi$ (-0.19 v=2) + $1^3\Pi$ (0.47 v=3)
2(II) v = 3	28921	28923		$1^1\Delta$ (-0.48 v=3) + $1^3\Delta$ (-0.74 v=3) + $1^3\Delta$ (-0.15 v=4) + $1^3\Pi$ (-0.21 v=3) + $1^3\Pi$ (0.37 v=4)
2(II) v = 4	29833	29830		$1^1\Delta$ (-0.51 v=4) + $1^3\Delta$ (-0.77 v=4) + $1^3\Delta$ (0.12 v=5) + 1 $^3\Pi$ (-0.22 v=4) +$1^3\Pi$ (0.27 v=5)
2(III) v = 0	28012	28013		$1^1\Delta$ (-0.84 v=0) + $1^3\Delta$ (0.46 v=0) + $1^3\Pi$ (0.25 v=0)
2(III) v = 1	29090	29092		$1^1\Delta$ (-0.85 v=1) + $1^3\Delta$ (0.46 v=1) + $1^3\Pi$ (0.25 v=1)
2(III) v = 2	30113	30114		$1^1\Delta$ (0.84 v=2) +$1^3\Delta$ (0.46 v=2)+ $1^3\Pi$ (-0.26 v=2)
2(III) v = 3	31073	31075		$1^1\Delta$ (0.84 v=3) + $1^3\Delta$ (-0.47 v=3) + $1^3\Pi$ (-0.26 v=3)
2(III) v = 4	31968	31966		$1^1\Delta$ (-0.81 v=4) + $1^3\Delta$ (0.46 v=4) +$1^3\Pi$ (0.26 v=4)
3(I) v = 0	25357	25357		$1^3\Delta$ (1 v=0)
3(I) v = 1	26447	26447		$1^3\Delta$ (1 v=1)
3(I) v = 2	27482	27482		$1^3\Delta$ (1 v=2)
3(I) v = 3	28463	28463		$1^3\Delta$ (1 v=3)
3(I) v = 4	29382	29382		$1^3\Delta$ (1 v=4)
3(I) v = 5	30234	30234		$1^3\Delta$ (1 v=5)
3(I) v = 6	31008	31008		$1^3\Delta$ (1 v=6)
3(I) v = 7	31687	31687		$1^3\Delta$ (1 v=7)
3(I) v = 8	32250	32250		$1^3\Delta$ (1 v=8)
3(I) v = 9	32668	32668		$1^3\Delta$ (1 v=9)
3(I) v = 10	32888	32888		$1^3\Delta$ (1 v=10)

Table S17

Spin-orbit matrix elements (in cm^{-1}) between vibrational levels of the $A^1\Sigma^+$ and $1^3\Pi$ states of CuH.

$\left\langle \psi_{vib,l} \left| \left\langle \psi_{el,i} \left| \hat{\mathbf{H}}_{\mathbf{SO}} \right| \psi_{el,j} \right\rangle \right| \psi_{vib,m} \right\rangle$

		$\mathbf{A^1\Sigma^+}$								
		v = 0	v = 1	v = 2	v = 3	v = 4	v = 5	v = 6	v = 7	v = 8
$\mathbf{1^3\Pi}$	v = 0	-800.73	269.20	-21.38	-1.33	-0.62	-0.36	0.01	0.23	0.20
	v = 1	216.52	731.19	-381.64	42.07	3.14	-0.25	-0.36	0.11	0.22
	v = 2	-73.69	-287.58	-655.76	471.62	-58.32	-6.33	-2.05	-0.10	0.48
	v = 3	29.75	119.36	328.10	578.16	-547.71	80.66	7.20	1.75	1.55
	v = 4	-13.72	-56.21	-163.29	-342.07	-499.03	621.98	-106.70	-17.89	-2.73
	v = 5	6.97	29.83	85.53	193.91	335.43	412.72	-696.32	127.35	37.08
	v = 6	-3.89	-17.16	-48.22	-111.89	-208.81	-305.42	-301.59	779.02	-108.88
	v = 7	2.18	9.59	26.82	62.03	120.50	185.36	221.94	173.87	-887.23

Table S18

Spin-orbit matrix elements (in cm^{-1}) between vibrational levels of the $A^1\Sigma^+$ and $1^3\Pi$ states of CuD.

$\left\langle \psi_{vib,l} \left| \left\langle \psi_{el,i} \left| \hat{\mathbf{H}}_{\mathbf{SO}} \right| \psi_{el,j} \right\rangle \right| \psi_{vib,m} \right\rangle$

		$\mathbf{A^1\Sigma^+}$									
		v = 0	v = 1	v = 2	v = 3	v = 4	v = 5	v = 6	v = 7	v = 8	v = 9
$\mathbf{1^3\Pi}$	v = 0	-785.44	305.38	-42.68	-0.24	-0.74	0.21	0.57	0.30	0.00	-0.10
	v = 1	256.34	688.29	-420.35	79.86	-2.49	-0.07	0.40	-0.39	-0.69	-0.28
	v = 2	-91.73	-329.43	-587.59	507.10	-116.95	2.12	2.26	0.28	-0.83	-0.41
	v = 3	36.01	144.89	369.57	484.75	-572.71	147.68	-0.67	-0.60	-1.25	0.04
	v = 4	-15.13	-67.39	-191.62	-378.10	-390.08	620.59	-186.52	2.80	-0.93	0.11
	v = 5	7.04	33.95	100.53	229.07	365.53	298.32	-659.82	231.48	-3.97	-0.55
	v = 6	-3.83	-18.13	-56.04	-132.90	-248.40	-340.06	-208.18	692.58	-281.38	0.59
	v = 7	2.46	10.31	33.11	78.80	157.71	257.95	297.37	113.64	-716.26	334.79
	v = 8	-1.73	-6.33	-20.32	-48.63	-100.37	-177.56	-249.36	-239.60	-12.49	729.79
	v = 9	1.22	4.13	12.70	30.92	64.83	118.28	184.06	217.37	156.19	-86.32

Table S19

Transition dipole moments for the Ω = 0^+(II), 0^+(III), 1(I), 1(II), 1(III), 1(IV), and 1(V) states of CuH in Debye (D).

r (Å)	0^+(II) → 0^+(I)	0^+(III) → 0^+(I)	1(I) → 0^+(I)	1(II) → 0^+(I)	1(III) → 0^+(I)	1(IV) → 0^+(I)	1(V) → 0^+(I)
1.00	2.91795	0.16505	0.01414	0.08550	-0.07321	0.69053	0.01414
1.05	2.74590	0.18791	0.01703	0.10271	-0.06156	0.69227	0.01414
1.10	2.58130	0.21267	0.01975	0.12321	-0.04183	0.69255	0.01414
1.15	2.43017	0.23826	0.02280	0.14269	0.01000	0.69103	0.01414
1.20	2.26503	0.26298	0.02588	0.15652	0.03017	0.68767	0.01414
1.25	2.11088	0.28721	0.02915	0.16374	0.07490	0.68162	0.01449
1.30	1.95137	0.30897	0.03225	0.16685	0.11962	0.67262	0.01483
1.35	1.90002	0.34104	0.03521	0.16888	0.16199	0.66098	0.01517
1.40	1.82594	0.36643	0.03821	0.17097	0.20487	0.64502	0.01612
1.45	1.75539	0.39812	0.04087	0.17231	0.24570	0.62540	0.01703
1.46	1.74142	0.39564	0.04147	0.17274	0.25371	0.62104	0.01732
1.47	1.72191	0.41095	0.04195	0.17315	0.26083	0.61690	0.01761
1.50	1.67269	0.42659	0.04347	0.17459	0.28406	0.60273	0.01871
1.55	1.59552	0.45252	0.04572	0.17649	0.31741	0.57864	0.02049
1.60	1.52204	0.47556	0.04775	0.17872	0.34383	0.55456	0.02345
1.65	1.45443	0.49549	0.04940	0.18125	0.35937	0.53426	0.02665
1.70	1.38813	0.51362	0.05070	0.18325	0.38240	0.50629	0.03162
1.75	1.32538	0.52690	0.05167	0.18566	0.38839	0.48808	0.03873
1.80	1.26792	0.53843	0.05206	0.18722	0.39695	0.46358	0.04930
1.90	1.15408	0.56721	0.05148	0.18818	0.40165	0.41276	0.09818
2.00	1.05586	0.57074	0.04785	0.18724	0.38324	0.32419	0.21640
2.10	0.96594	0.57001	0.03912	0.17026	0.25280	0.35702	0.19942
2.20	0.67130	0.42994	0.02191	0.09644	0.18000	0.24962	0.15937
2.30	0.41076	0.27968	0.00949	0.01414	0.16100	0.18871	0.09241
2.40	0.28358	0.20100	0.00447	-0.01225	0.13528	0.15277	0.06356
2.50	0.18788	0.13667	0.00000	-0.01643	0.11432	0.12450	0.03924
2.60	0.11870	0.08729	0.00000	-0.02530	0.09257	0.09975	0.03435
2.70	0.06557	0.04817	0.00000	-0.02236	0.07707	0.07981	0.02429
2.80	0.02881	0.02098	0.00000	-0.02214	0.06197	0.06387	0.01817
2.90	0.00447	0.00316	0.00000	-0.01975	0.05060	0.05225	0.00949
3.00	0.01140	0.00775	0.00000	-0.01761	0.04025	0.04207	0.00316
3.20	0.02280	0.01643	0.00000	-0.01342	0.02569	0.02683	0.00000
3.40	0.02098	0.01517	0.00000	-0.00949	0.01612	0.01703	0.00000
3.60	0.01517	0.01095	0.00707	0.00000	0.01049	0.01095	0.00316
3.80	0.00949	0.00707	0.00447	0.00000	0.00707	0.00447	0.00548
4.00	0.00548	0.00316	0.00548	0.00000	0.00447	0.00000	0.00447
4.50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5.50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6.50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7.50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8.50	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Table S20

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 0^+(II) → 0^+(I) transition of CuH.

	0^+(II)									
	$A_{v'\to v''}$									
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7	v′ = 8
0^+(I)	v″ = 0	7.82E+06	3.03E+06	9.53E+05	2.82E+05	8.46E+04	2.71E+04	9.73E+03	3.73E+03	1.07E+03
	v″ = 1	1.14E+06	3.79E+06	3.70E+06	1.81E+06	7.51E+05	3.05E+05	1.29E+05	5.35E+04	1.56E+04
	v″ = 2	2.55E+04	1.74E+06	1.54E+06	3.16E+06	2.26E+06	1.24E+06	6.29E+05	2.91E+05	8.91E+04
	v″ = 3	3.78E+01	7.43E+04	1.94E+06	3.94E+05	2.15E+06	2.17E+06	1.51E+06	8.30E+05	2.75E+05
	v″ = 4	5.14E+00	2.31E+02	1.38E+05	1.86E+06	6.23E+03	1.09E+06	1.56E+06	1.20E+06	4.63E+05
	v″ = 5	1.34E+00	1.59E+01	8.91E+02	2.22E+05	1.48E+06	1.72E+05	2.78E+05	6.77E+05	3.57E+05
	v″ = 6	3.03E-01	3.16E+00	5.25E+01	2.37E+03	2.92E+05	7.94E+05	5.87E+05	1.14E+04	2.29E+04
	v″ = 7	3.46E-02	8.41E-01	3.21E+01	7.39E-01	1.77E+03	2.76E+05	1.95E+05	5.15E+05	1.75E+05
	v″ = 8	3.67E-04	1.40E+00	3.06E+00	4.29E+02	8.89E+02	1.08E+03	2.10E+05	6.96E+00	4.30E+04

Table S21

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 0^+(III) → 0^+(I) transition of CuH.

	0^+(III)					
	$A_{v'\to v''}$					
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4
0^+(I)	v″ = 0	6.35E+05	2.79E+05	9.70E+04	3.26E+04	1.13E+04
	v″ = 1	4.30E+05	1.22E+05	2.31E+05	1.45E+05	7.09E+04
	v″ = 2	7.51E+04	5.31E+05	1.38E+02	1.05E+05	1.25E+05
	v″ = 3	3.25E+03	1.86E+05	4.48E+05	5.25E+04	1.83E+04
	v″ = 4	1.92E+01	1.36E+04	3.01E+05	2.71E+05	1.51E+05
	v″ = 5	8.87E-01	1.54E+02	3.19E+04	3.74E+05	8.27E+04
	v″ = 6	1.47E-02	2.32E+00	3.59E+02	5.56E+04	3.40E+05
	v″ = 7	7.85E-01	1.87E+00	5.39E+01	2.37E+02	6.57E+04
	v″ = 8	2.62E-01	6.63E-01	3.11E+01	5.96E+02	9.91E+00

Table S22

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(I) → 0^+(I) transition of CuH.

	1(I)			
	$A_{v'\to v''}$			
		v′ = 0	v′ = 1	v′ = 2
0^+(I)	v″ = 0	3.57E+03	3.93E+02	3.00E+01
	v″ = 1	6.79E+02	2.39E+03	7.58E+02
	v″ = 2	2.22E+01	1.25E+03	1.08E+03
	v″ = 3	1.01E-01	8.32E+01	1.54E+03
	v″ = 4	3.50E-03	1.44E+00	2.34E+02
	v″ = 5	5.76E-05	6.67E-02	1.48E+01
	v″ = 6	2.00E-05	8.17E-04	1.03E+00
	v″ = 7	2.49E-07	1.14E-03	3.34E-04
	v″ = 8	5.55E-06	1.93E-04	2.81E-02

Table S23

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(II) → 0^+(I) transition of CuH.

	1(II)								
	$A_{v'\to v''}$								
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7
0^+(I)	v″ = 0	8.32E+04	4.79E+04	2.15E+04	9.13E+03	3.91E+03	1.79E+03	7.95E+02	2.35E+02
	v″ = 1	4.92E+04	1.21E+04	3.44E+04	2.77E+04	1.66E+04	9.36E+03	4.75E+03	1.51E+03
	v″ = 2	8.39E+03	5.59E+04	3.38E+02	1.18E+04	1.85E+04	1.59E+04	1.01E+04	3.55E+03
	v″ = 3	4.45E+02	2.00E+04	4.04E+04	1.07E+04	3.87E+02	5.31E+03	6.67E+03	3.06E+03
	v″ = 4	5.36E+00	1.75E+03	2.98E+04	1.72E+04	2.15E+04	3.68E+03	5.83E+00	1.56E+02
	v″ = 5	1.91E-03	2.89E+01	3.91E+03	3.11E+04	6.23E+02	1.71E+04	1.18E+04	2.98E+03
	v″ = 6	1.17E-02	4.21E-01	4.63E+01	5.52E+03	1.69E+04	6.38E+03	5.55E+02	1.94E+03
	v″ = 7	1.37E-02	1.19E+00	2.57E+01	8.83E-06	4.01E+03	2.34E+03	7.36E+03	2.48E+03
	v″ = 8	3.02E-03	3.72E-01	1.63E+01	2.29E+02	1.29E+02	2.16E+03	2.37E+01	2.55E+02

Table S24

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(III) → 0^+(I) transition of CuH.

	1(III)							
	$A_{v'\to v''}$							
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6
0^+(I)	v″ = 0	3.20E+05	1.20E+05	2.74E+04	5.96E+03	1.50E+03	2.20E+02	1.97E+01
	v″ = 1	2.68E+05	4.25E+04	9.07E+04	4.85E+04	2.63E+04	9.19E+03	1.81E+03
	v″ = 2	5.49E+04	2.90E+05	7.68E+03	1.70E+04	3.94E+04	2.78E+04	7.71E+03
	v″ = 3	2.89E+03	1.29E+05	1.54E+05	8.97E+04	9.53E+03	1.88E+03	2.61E+03
	v″ = 4	4.89E+01	1.22E+04	1.70E+05	4.05E+03	9.69E+04	6.50E+04	1.25E+04
	v″ = 5	6.83E-02	2.60E+02	3.03E+04	8.49E+04	4.55E+04	1.05E+03	6.43E+03
	v″ = 6	1.60E+00	7.45E+00	9.44E+02	3.81E+04	9.74E+03	4.19E+04	1.15E+04
	v″ = 7	9.30E-02	2.05E+01	1.24E+01	4.22E+03	2.78E+04	2.31E+03	8.32E+02
	v″ = 8	1.20E-02	2.57E+00	5.48E+00	4.20E+02	8.23E+03	6.66E+03	4.75E+03

Table S25

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(IV) → 0^+(I) transition of CuH.

	1(IV)							
	$A_{v'\to v''}$							
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6
0^+(I)	v″ = 0	1.12E+06	8.42E+05	4.67E+05	2.38E+05	1.10E+05	5.30E+04	2.06E+04
	v″ = 1	5.58E+05	8.59E+04	4.69E+05	5.20E+05	3.60E+05	2.24E+05	1.00E+05
	v″ = 2	7.16E+04	5.25E+05	4.31E+04	9.18E+04	2.50E+05	2.62E+05	1.49E+05
	v″ = 3	2.60E+03	1.54E+05	2.72E+05	2.08E+05	7.09E+03	2.77E+04	4.81E+04
	v″ = 4	1.61E+01	9.73E+03	1.95E+05	7.20E+04	2.02E+05	9.84E+04	2.02E+04
	v″ = 5	9.23E-01	1.09E+02	2.22E+04	1.92E+05	1.17E+02	8.66E+04	7.43E+04
	v″ = 6	6.70E-02	4.49E+00	1.05E+03	4.20E+04	1.16E+05	5.10E+04	2.18E+02
	v″ = 7	1.04E+00	2.42E+01	1.20E+02	2.73E+03	4.79E+04	1.66E+04	3.85E+04
	v″ = 8	5.65E-03	5.79E-02	8.47E-01	1.45E+00	4.14E+03	3.41E+04	3.69E+03

Table S26

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(V) → 0^+(I) transition of CuH.

	1(V)					
	$A_{v'\to v''}$					
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4
0^+(I)	v″ = 0	3.89E+03	1.17E+04	1.46E+04	1.22E+04	5.40E+03
	v″ = 1	5.72E+04	1.01E+05	7.49E+04	3.97E+04	1.27E+04
	v″ = 2	3.51E+05	2.76E+05	7.63E+04	1.06E+04	4.53E+02
	v″ = 3	1.17E+06	1.84E+05	3.40E+03	3.91E+04	2.35E+04
	v″ = 4	2.31E+06	6.46E+04	2.67E+05	1.06E+05	1.91E+04
	v″ = 5	2.71E+06	1.93E+06	1.51E+05	1.70E+04	3.24E+04
	v″ = 6	1.83E+06	5.45E+06	7.38E+05	6.06E+05	1.05E+05
	v″ = 7	6.39E+05	5.94E+06	7.43E+06	1.45E+05	9.92E+04
	v″ = 8	9.50E+04	2.97E+06	1.53E+07	3.05E+06	1.78E+06

Table S27

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 0^+(II) → 0^+(I) transition of CuD.

	0^+(II)									
	$A_{v'\to v''}$									
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7	v′ = 8
0^+(I)	v″ = 0	7.16E+06	3.39E+06	1.20E+06	3.69E+05	1.04E+05	2.95E+04	8.92E+03	3.16E+03	1.40E+03
	v″ = 1	1.79E+06	2.63E+06	3.78E+06	2.17E+06	9.25E+05	3.64E+05	1.42E+05	5.74E+04	2.47E+04
	v″ = 2	1.09E+05	2.49E+06	6.41E+05	2.89E+06	2.53E+06	1.49E+06	7.58E+05	3.67E+05	1.75E+05
	v″ = 3	1.51E+03	2.87E+05	2.49E+06	2.83E+04	1.71E+06	2.37E+06	1.85E+06	1.17E+06	6.64E+05
	v″ = 4	1.94E+01	6.75E+03	4.69E+05	2.15E+06	1.07E+05	7.22E+05	1.78E+06	1.86E+06	1.42E+06
	v″ = 5	2.32E-02	5.81E+01	1.71E+04	6.45E+05	1.60E+06	4.79E+05	1.45E+05	1.02E+06	1.48E+06
	v″ = 6	3.00E-01	8.07E-01	1.79E+02	3.21E+04	8.18E+05	9.64E+05	8.41E+05	3.15E+03	3.60E+05
	v″ = 7	1.67E-01	2.39E-01	1.57E-02	8.16E+02	6.13E+04	9.23E+05	3.86E+05	1.02E+06	1.85E+05
	v″ = 8	8.62E-03	1.59E-02	5.55E+00	4.56E+00	2.35E+03	9.81E+04	8.63E+05	3.91E+04	8.53E+05

Table S28

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 0^+(III) → 0^+(I) transition of CuD.

	0^+(III)									
	$A_{v'\to v''}$									
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7	v′ = 8
0^+(I)	v″ = 0	5.05E+05	3.19E+05	1.44E+05	5.78E+04	2.23E+04	8.56E+03	3.24E+03	1.22E+03	4.65E+02
	v″ = 1	4.79E+05	2.30E+04	1.78E+05	1.70E+05	1.04E+05	5.46E+04	2.68E+04	1.29E+04	6.22E+03
	v″ = 2	1.45E+05	4.37E+05	3.85E+04	3.56E+04	1.06E+05	1.06E+05	7.57E+04	4.65E+04	2.69E+04
	v″ = 3	1.63E+04	2.99E+05	2.45E+05	1.41E+05	1.02E+03	3.31E+04	6.90E+04	7.00E+04	5.40E+04
	v″ = 4	5.74E+02	5.56E+04	4.00E+05	7.82E+04	1.80E+05	3.99E+04	4.21E+02	2.19E+04	3.86E+04
	v″ = 5	1.01E+01	3.39E+03	1.17E+05	4.20E+05	2.89E+03	1.44E+05	8.92E+04	1.58E+04	1.12E+02
	v″ = 6	2.19E+00	6.69E+01	9.99E+03	1.88E+05	3.52E+05	2.45E+04	6.82E+04	9.98E+04	5.04E+04
	v″ = 7	3.54E-01	1.62E+00	1.98E+02	2.19E+04	2.60E+05	2.19E+05	1.10E+05	8.15E+03	6.51E+04
	v″ = 8	1.39E-01	1.82E+00	7.40E-02	6.38E+02	4.06E+04	2.91E+05	7.04E+04	1.86E+05	1.60E+04

Table S29

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(I) → 0^+(I) transition of CuD.

	1(I)			
	$A_{v'\to v''}$			
		v′ = 0	v′ = 1	v′ = 2
0^+(I)	v″ = 0	3.37E+03	5.44E+02	6.28E+01
	v″ = 1	8.58E+02	2.00E+03	9.10E+02
	v″ = 2	5.50E+01	1.48E+03	8.98E+02
	v″ = 3	1.02E+00	1.74E+02	1.78E+03
	v″ = 4	1.41E-02	6.03E+00	3.67E+02
	v″ = 5	5.04E-04	1.63E-01	2.44E+01
	v″ = 6	1.91E-06	9.37E-03	1.35E+00
	v″ = 7	1.91E-05	1.64E-04	1.09E-01
	v″ = 8	8.26E-07	9.80E-06	4.85E-03

Table S30

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(II) → 0^+(I) transition of CuD.

	1(II)									
	$A_{v'\to v''}$									
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7	v′ = 8
0^+(I)	v″ = 0	6.56E+04	5.13E+04	2.81E+04	1.36E+04	6.22E+03	2.83E+03	1.32E+03	6.65E+02	3.30E+02
	v″ = 1	5.70E+04	1.44E+03	2.40E+04	2.95E+04	2.22E+04	1.39E+04	8.00E+03	4.70E+03	2.60E+03
	v″ = 2	1.70E+04	4.64E+04	7.77E+03	3.00E+03	1.50E+04	1.86E+04	1.57E+04	1.18E+04	7.74E+03
	v″ = 3	2.08E+03	3.31E+04	2.08E+04	2.09E+04	1.19E+03	2.56E+03	8.31E+03	1.08E+04	9.68E+03
	v″ = 4	1.06E+02	6.87E+03	4.03E+04	3.56E+03	2.15E+04	9.00E+03	5.60E+02	7.53E+02	2.95E+03
	v″ = 5	2.29E+00	5.35E+02	1.37E+04	3.67E+04	4.83E+02	1.18E+04	1.32E+04	6.00E+03	1.24E+03
	v″ = 6	2.75E-02	1.58E+01	1.51E+03	2.07E+04	2.40E+04	8.52E+03	1.75E+03	9.08E+03	8.31E+03
	v″ = 7	2.29E-05	1.12E-01	5.67E+01	3.20E+03	2.48E+04	7.42E+03	1.78E+04	1.65E+03	1.29E+03
	v″ = 8	5.98E-04	9.25E-03	1.17E-01	1.25E+02	5.09E+03	2.03E+04	6.25E+01	1.30E+04	1.04E+04

Table S31

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(III) → 0^+(I) transition of CuD.

	1(III)									
	$A_{v'\to v''}$									
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7	v′ = 8
0^+(I)	v″ = 0	2.55E+07	1.45E+05	5.03E+04	1.34E+04	3.64E+03	1.23E+03	3.19E+02	7.62E+01	1.76E+01
	v″ = 1	2.85E+05	5.56E+03	7.52E+04	6.00E+04	3.04E+04	1.72E+04	7.53E+03	2.94E+03	1.03E+03
	v″ = 2	9.97E+04	2.28E+05	3.61E+04	6.63E+03	2.58E+04	3.36E+04	2.57E+04	1.49E+04	6.91E+03
	v″ = 3	1.33E+04	1.93E+05	8.95E+04	9.34E+04	1.49E+04	1.21E+02	8.93E+03	1.40E+04	1.04E+04
	v″ = 4	7.66E+02	4.41E+04	2.23E+05	2.78E+03	6.65E+04	6.34E+04	1.99E+04	1.92E+03	4.28E+01
	v″ = 5	2.41E+01	3.90E+03	8.97E+04	1.51E+05	4.66E+04	4.42E+03	4.82E+04	4.36E+04	1.97E+04
	v″ = 6	7.36E-02	1.99E+02	1.22E+04	1.22E+05	1.56E+04	1.05E+05	3.18E+04	3.54E+02	1.01E+04
	v″ = 7	9.92E-02	1.10E+00	6.73E+02	2.87E+04	7.34E+04	2.03E+04	2.61E+04	6.08E+04	2.96E+04
	v″ = 8	4.08E-02	4.43E+00	4.61E-03	2.62E+03	3.80E+04	1.12E+04	4.59E+04	4.38E+03	3.26E+03

Table S32

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(IV) → 0^+(I) transition of CuD.

	1(IV)									
	$A_{v'\to v''}$									
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6	v′ = 7	v′ = 8
0^+(I)	v″ = 0	8.84E+05	8.52E+05	5.48E+05	3.14E+05	1.67E+05	8.08E+04	4.20E+04	2.08E+04	1.04E+04
	v″ = 1	6.94E+05	1.80E+03	2.87E+05	4.80E+05	4.54E+05	3.15E+05	2.09E+05	1.23E+05	6.91E+04
	v″ = 2	1.78E+05	4.60E+05	1.74E+05	5.34E+03	1.71E+05	2.88E+05	3.05E+05	2.41E+05	1.62E+05
	v″ = 3	1.85E+04	3.13E+05	1.27E+05	3.11E+05	7.27E+04	4.48E+03	7.86E+04	1.36E+05	1.34E+05
	v″ = 4	8.15E+02	5.79E+04	3.15E+05	4.04E+02	2.20E+05	1.91E+05	5.02E+04	2.72E+02	1.01E+04
	v″ = 5	1.58E+01	4.03E+03	1.03E+05	2.11E+05	4.86E+04	5.02E+04	1.70E+05	1.34E+05	5.81E+04
	v″ = 6	4.04E-04	6.85E+01	1.07E+04	1.33E+05	9.98E+04	1.11E+05	1.30E+03	3.84E+04	7.38E+04
	v″ = 7	6.03E-01	1.89E-01	4.28E+02	2.26E+04	1.47E+05	1.96E+04	1.25E+05	4.59E+04	1.76E+03
	v″ = 8	7.11E-02	2.87E+00	4.84E+01	2.08E+03	4.16E+04	1.21E+05	7.16E+03	5.12E+04	7.27E+04

Table S33

Einstein A coefficients ($A_{v'\to v''}$ in s^{-1}) for the 1(V) → 0^+(I) transition of CuD.

	1(V)							
	$A_{v'\to v''}$							
		v′ = 0	v′ = 1	v′ = 2	v′ = 3	v′ = 4	v′ = 5	v′ = 6
0^+(I)	v″ = 0	2.76E+02	1.50E+03	3.64E+03	5.30E+03	5.68E+03	4.60E+03	2.15E+03
	v″ = 1	5.24E+03	2.01E+04	3.39E+04	3.53E+04	2.77E+04	1.73E+04	6.81E+03
	v″ = 2	4.40E+04	1.08E+05	1.11E+05	6.84E+04	3.01E+04	1.03E+04	2.49E+03
	v″ = 3	2.15E+05	2.84E+05	1.28E+05	2.19E+04	1.83E+01	3.46E+03	3.28E+03
	v″ = 4	6.76E+05	3.34E+05	1.14E+04	2.62E+04	5.23E+04	3.67E+04	1.34E+04
	v″ = 5	1.44E+06	6.65E+04	1.27E+05	1.54E+05	4.99E+04	5.55E+03	3.83E+01
	v″ = 6	2.09E+06	2.27E+05	3.97E+05	3.18E+04	1.74E+04	4.58E+04	2.48E+04
	v″ = 7	2.04E+06	1.87E+06	5.07E+04	1.74E+05	1.73E+05	5.63E+04	9.23E+03
	v″ = 8	1.29E+06	3.80E+06	8.42E+05	4.62E+05	3.05E+03	3.92E+04	3.33E+04

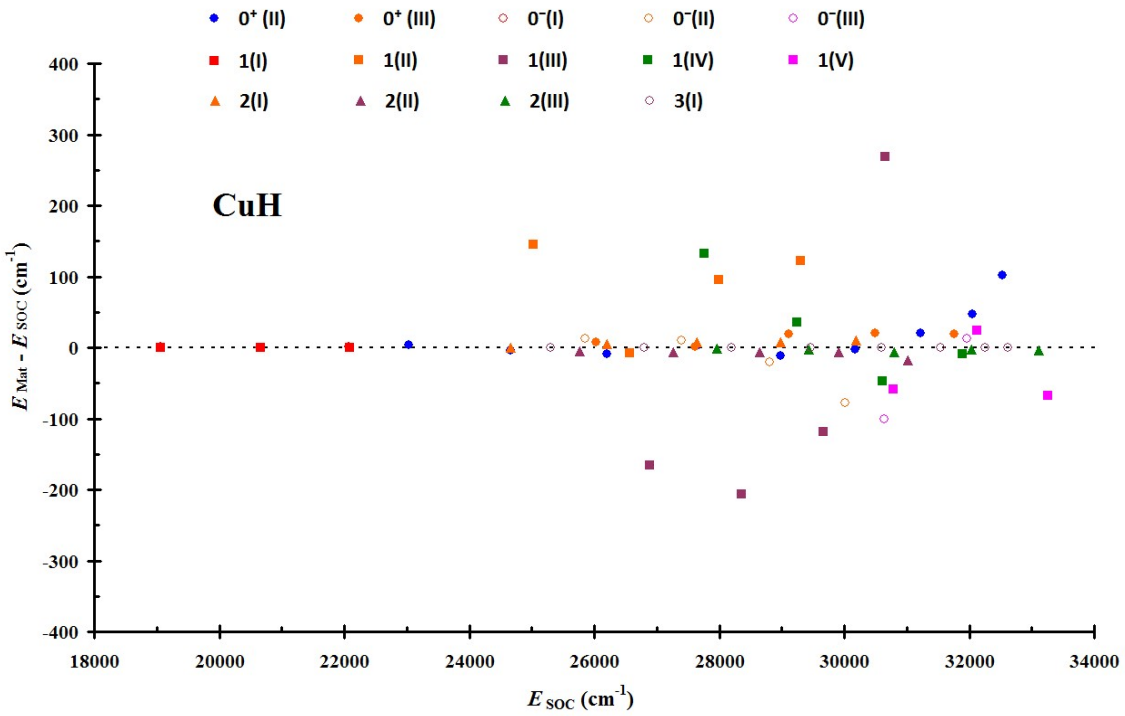

Figure S1. The differences in vibronic energies calculated by two different SOC methods for CuH.

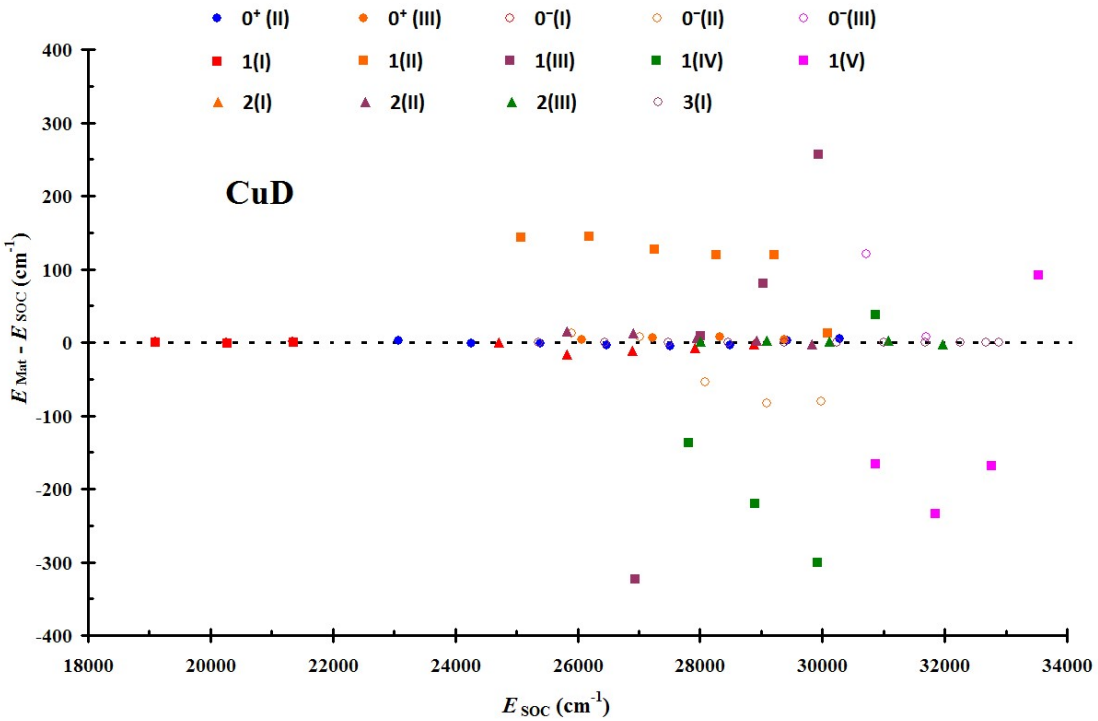

Figure S2. The differences in vibronic energies calculated by two different SOC methods for CuD.