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Can a Linear Metal–Metal Bonded Array of Tetravanadium Be Stabilized between Two Dicyclopenta[a,e]pentalene Ligands? A Theoretical Investigation

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(1) Diagrams for molecular orbitals

(2) The bond distances and the bond indices for vanadium-carbon

(3) Gibbs free energy change in the related reference reactions

(4) List of the Cartesian coordinates and the lowest five frequencies for studied complexes

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(1) Diagrams for molecular orbitals

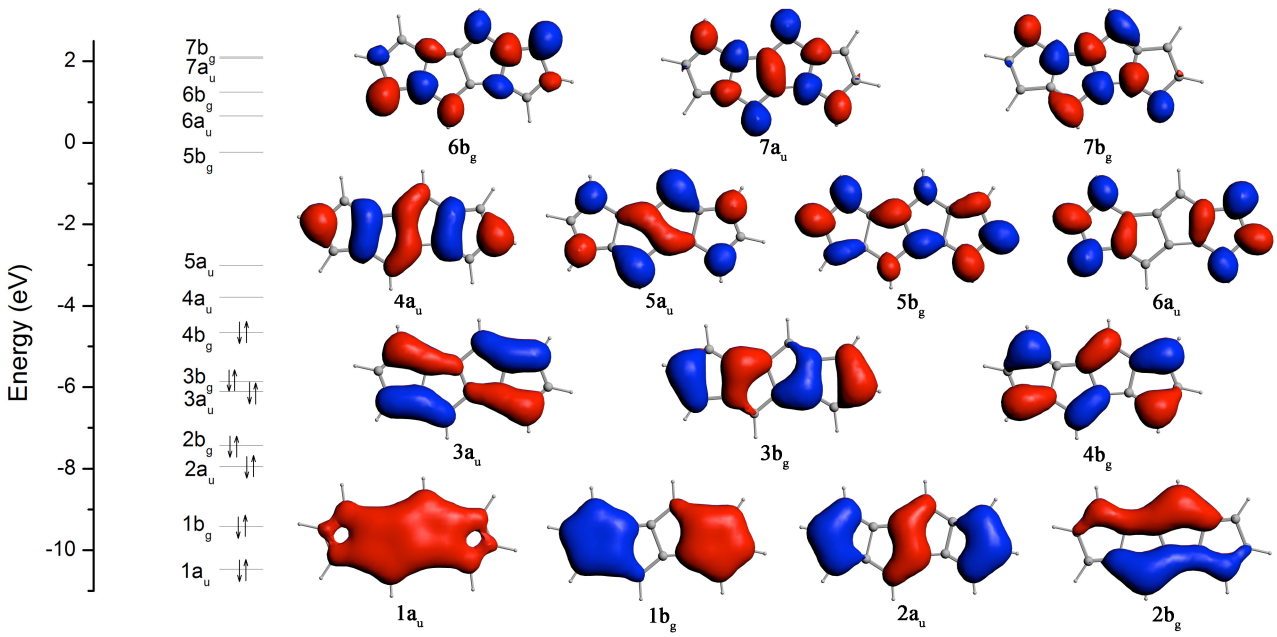

Fig. S1 The frontier molecular orbitals (FMOs) within π symmetry and their energy levels for dcpp.

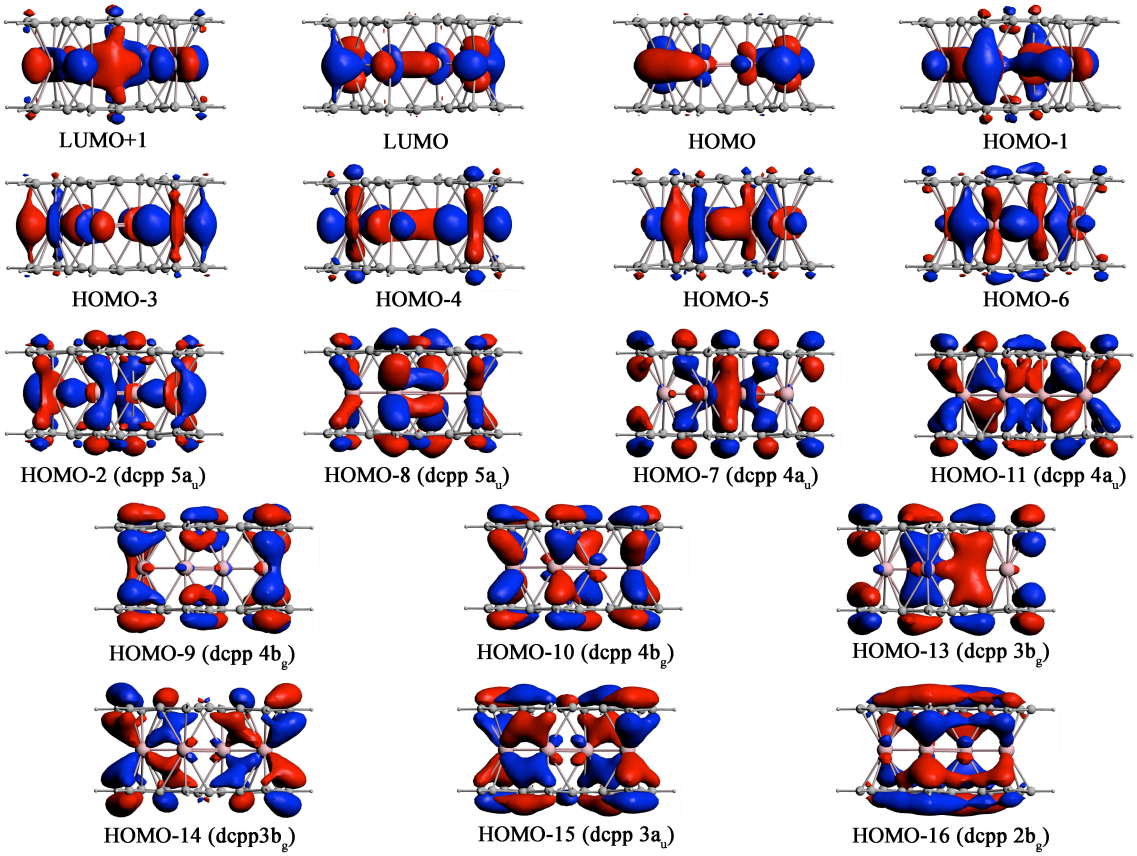

Fig. S2 The FMOs of **1a-S** with explicit contribitons from the occupied dcpp ligand orbitals (HOMO-16, HOMO-15, HOMO-14, HOMO-13, HOMO-10 and HOMO-9), from the unoccupied dcpp ligand orbitals (HOMO-11, HOMO-7, HOMO-8 and HOMO-2) and from almost only vanadium atoms. (The respective dcpp orbitals are labeled in the paratheses except for unoccupied complex FMOs)

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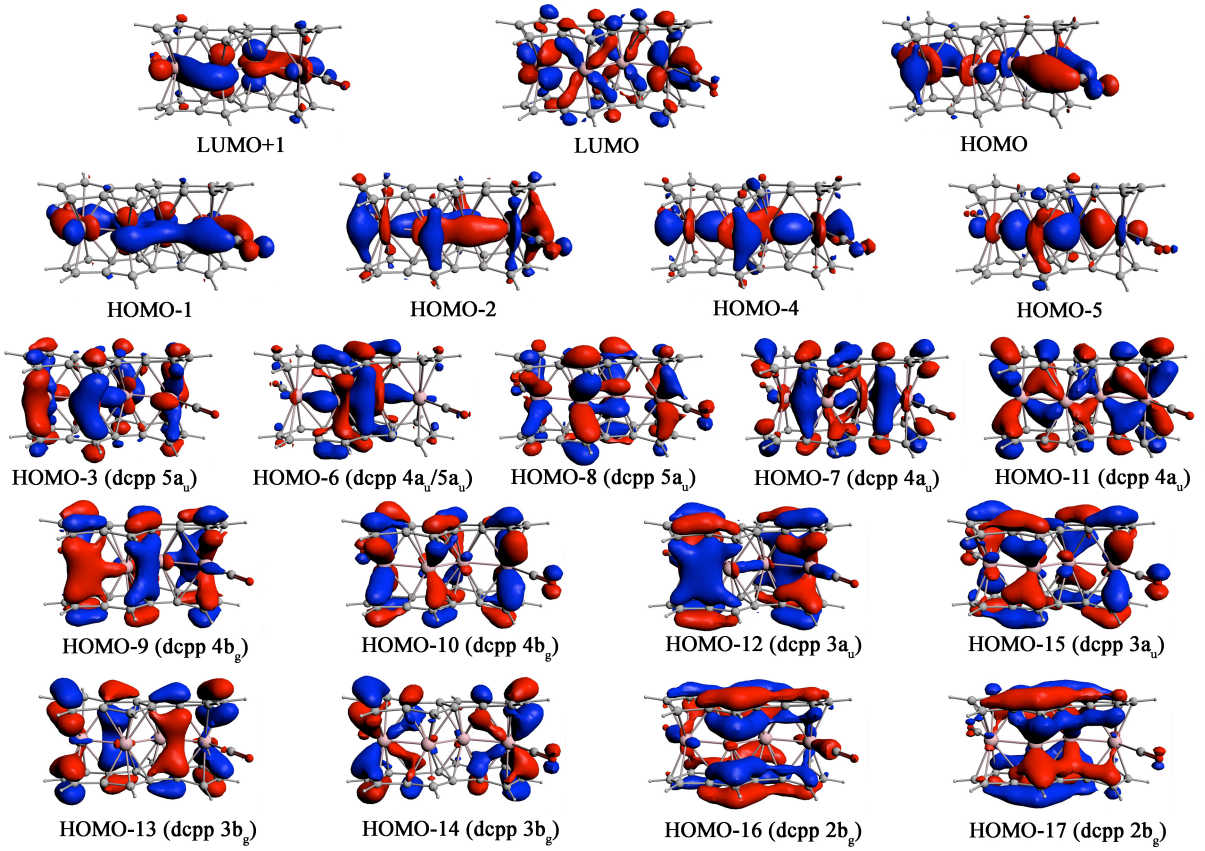

Fig. S3 The FMOs of **3a-cis-S** with explicit contribitons from the occupied dcpp ligand orbitals (HOMO-17, HOMO-16, HOMO-15, HOMO-14, HOMO-13, HOMO-12, HOMO-10 and HOMO-9), from the unoccupied dcpp ligand orbitals (HOMO-11, HOMO-7, HOMO-8, HOMO-6 and HOMO-3) and from almost only vanadium atoms. (The respective dcpp orbitals are labeled in the paratheses except for unoccupied complex FMOs)

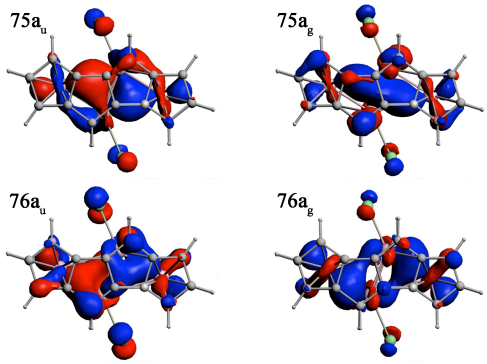

Fig. S4 The four occupied MOs related to the multicenter bonding of the tetravanadium moiety in $(dcpp)_2V_4Cl_2$. (only alpha spin orbitals shown)

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(2) The bond distances and the bond indices for vanadium-carbon

Table S1 The bond distances and the bond indices (whose print thredhold were set to 0.05) of all vanadium-carbon bonds in the selected minimum structures of $(dcpp)_2V_4$, $(dcpp)_2V_4Cl_2$ and $(dcpp)_2V_4(CO)_2$. (The data in the second low for each vanadium-carbon bond is for the carbon atom from the second dcpp ligand when they are different from the data for carbon atom from the first dcpp ligand. Based on these data, it could be concluded that delocalized interactions exist between vanadium-carbon.)

	1c-T		**2a-trans-T**		**2b-T**		**3a-cis-S**		**3b-T**	
	Bond distance	Bond index	Bond distance	Bond index	Bond distance	Bond index	Bond distance	Bond index	Bond distance	Bond index
V1-C1	2.257	0.31	2.324	0.41	2.245	0.36	2.244	0.40	2.251	0.34
					2.303	0.33			2.251	0.34
V1-C2	2.274	0.29	2.323	0.23	2.268	0.28	2.257	0.31	2.235	0.35
					2.272	0.31			2.235	0.35
V1-C3	2.281	0.30	2.325	0.40	2.286	0.37	2.326	0.40	2.271	0.38
					2.215	0.40			2.271	0.38
V1-C4	2.260	0.25	2.401	0.20	2.341	0.21	2.547	0.17	2.341	0.23
					2.205	0.27			2.341	0.23
V1-C14	2.245	0.256	2.453	0.21	2.273	0.23	2.384	0.20	2.276	0.28
					2.276	0.27			2.276	0.28
V2-C4	2.387	0.19	2.263	0.21	2.353	0.24	2.214	0.22	2.567	0.12
					2.952	0.07			2.568	0.12
V2-C5	2.055	0.68	2.151	0.49	2.141	0.45	2.148	0.47	2.202	0.41
					2.337	0.33			2.202	0.41
V2-C6	2.415	0.21	2.256	0.20	2.208	0.27	2.267	0.21	2.226	0.28
					2.410	0.18			2.226	0.28
V2-C13	2.980	–	2.443	0.18	2.557	0.13	2.323	0.21	2.545	0.15
					3.111	–			2.545	0.15
V2-C14	2.933	0.07	2.311	0.20	2.678	0.12	2.300	0.21	2.870	0.05
					3.325	–			2.870	0.05
V3-C6	2.290	0.26	2.443	0.18	3.111	–	2.323	0.21	3.167	–
					2.557	0.13			3.167	–
V3-C7	2.411	0.18	2.311	0.20	3.325	–	2.300	0.21	3.388	–
					2.678	0.12			3.388	–
V3-C11	2.355	0.20	2.263	0.21	2.952	0.07	2.214	0.22	2.779	0.07
					2.353	0.24			2.779	0.07
V3-C12	2.224	0.40	2.151	0.49	2.337	0.33	2.148	0.47	2.130	0.56
					2.141	0.45			2.130	0.56
V3-C13	2.237	0.28	2.256	0.20	2.410	0.18	2.267	0.21	2.414	0.16
					2.208	0.27			2.414	0.16
V4-C7	2.277	0.21	2.453	0.21	2.276	0.27	2.384	0.20	2.235	0.32
					2.273	0.23			2.235	0.32
V4-C8	2.250	0.36	2.324	0.41	2.303	0.33	2.244	0.40	2.219	0.36
					2.245	0.36			2.219	0.36
V4-C9	2.255	0.27	2.323	0.23	2.272	0.31	2.257	0.31	2.239	0.35
					2.268	0.28			2.239	0.35
V4-C10	2.223	0.39	2.325	0.40	2.215	0.40	2.326	0.40	2.315	0.33
					2.286	0.37			2.315	0.33
V4-C11	2.276	0.22	2.401	0.20	2.205	0.27	2.547	0.17	2.357	0.22
					2.341	0.21			2.357	0.22

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(3) Gibbs free energy change in the related reference reactions

Table S2 Gibbs free energy change (in kcal/mol) in the related reactions.

molecule	reference reaction	Δ_rG(gas)[a]	Δ_rG(THF)[b,c]	Δ_rG(n-hexane)[b,d]
Pn_2V_2	2 V + 2 Pn → Pn_2V_2	−308.8		
1c-T	4 V + 2 dcpp → **1c-T**	−550.9		
2b-T	4 V + 2 dcpp + Cl_2 → **2b-T**	−637.8		
	1c-T + Cl_2 → **2b-T**	−86.8	−86.4	−86.9
3a-cis-S	4 V + 2 dcpp + 2 CO → **3a-cis-S**	−548.5		
	1c-T + 2 CO → **3a-cis-S**	2.4	−4.0	−0.4
3b-T	4 V + 2 dcpp + 2 CO → **3b-T**	−563.2		
	1c-T + 2 CO → **3b-T**	−12.3	−20.2	−20.1

[a] The Gibbs free energy of atom vanadium was calculated based on the electronic configuration $3d^34s^2$. [b] The free energy in solution was calculated using the equation $G(soln) = G(gas) + \Delta G(1atm \rightarrow 1M) + \Delta G_{solv}$, where $\Delta G(1atm \rightarrow 1M)$ for the standard state transformation is 1.89 kcal/mol and ΔG_{solv} is the salvation free energy and was calculated via SMD[S1] parameterized PCM salvation model implemented in G09[S2] (at the level of B-VP86/def2-TZVPP[S3]). [c] Using the parameters for the solvent tetrahydrofuran. [d] Using the parameters for the solvent n-hexane.

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(4) List of the Cartesian coordinates and the lowest five frequencies:

1a-S

V	2.851490	-0.107331	0.000000
V	-2.851490	0.107331	0.000000
V	0.903134	0.753795	0.000000
V	-0.903134	-0.753795	0.000000
C	4.002135	-0.421687	-1.920924
C	2.915786	-1.359468	-1.850018
C	3.501023	0.910733	-1.923737
C	1.705832	-0.587768	-1.942844
C	2.060144	0.828956	-1.975021
C	4.002135	-0.421687	1.920924
C	3.501023	0.910733	1.923737
C	2.915786	-1.359468	1.850018
C	2.060144	0.828956	1.975021
C	1.705832	-0.587768	1.942844
H	5.054873	-0.691338	-1.910353
H	3.001351	-2.440033	-1.860360
H	4.096910	1.816398	-1.952796
H	5.054873	-0.691338	1.910353
H	4.096910	1.816398	1.952796
H	3.001351	-2.440033	1.860360
C	-0.253461	0.681188	-1.992618
C	0.835350	1.646597	-1.919157
C	0.253461	-0.681188	-1.992618
C	-0.253461	0.681188	1.992618
C	0.253461	-0.681188	1.992618
C	0.835350	1.646597	1.919157
H	0.766257	2.710288	-2.116577
H	0.766257	2.710288	2.116577
C	-2.060144	-0.828956	-1.975021
C	-1.705832	0.587768	-1.942844
C	-0.835350	-1.646597	-1.919157
C	-2.060144	-0.828956	1.975021
C	-0.835350	-1.646597	1.919157
C	-1.705832	0.587768	1.942844
H	-0.766257	-2.710288	-2.116577
H	-0.766257	-2.710288	2.116577
C	-4.002135	0.421687	-1.920924
C	-2.915786	1.359468	-1.850018
C	-3.501023	-0.910733	-1.923737
C	-4.002135	0.421687	1.920924

C	-3.501023	-0.910733	1.923737
C	-2.915786	1.359468	1.850018
H	-3.001351	2.440033	-1.860360
H	-3.001351	2.440033	1.860360
H	-5.054873	0.691338	-1.910353
H	-5.054873	0.691338	1.910353
H	-4.096910	-1.816398	-1.952796
H	-4.096910	-1.816398	1.952796

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
-84.682118	35.149944	-0.746095
86.271094	2.367576	0.051197
104.062825	0.000000	0.000000
125.696235	0.000000	0.000000
134.596906	30.119241	1.016148

1a-T

V	2.725004	-0.190458	0.000000
V	-2.725004	0.190458	0.000000
V	-0.766498	-0.861677	0.000000
V	0.766498	0.861677	0.000000
C	3.988708	-0.446230	-1.863595
C	2.894533	-1.371389	-1.917753
C	3.494853	0.891318	-1.831102
C	1.698309	-0.594472	-2.000141
C	2.057577	0.825085	-1.945700
C	3.988708	-0.446230	1.863595
C	3.494853	0.891318	1.831102
C	2.894533	-1.371389	1.917753
C	2.057577	0.825085	1.945700
C	1.698309	-0.594472	2.000141
H	5.037571	-0.725748	-1.823282
H	2.975790	-2.452686	-1.946198
H	4.101587	1.789805	-1.790096
H	5.037571	-0.725748	1.823282
H	4.101587	1.789805	1.790096

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H	2.975790	-2.452686	1.946198
C	-0.249516	0.676783	-2.085944
C	0.831130	1.651482	-1.952902
C	0.249516	-0.676783	-2.085944
C	-0.249516	0.676783	2.085944
C	0.249516	-0.676783	2.085944
C	0.831130	1.651482	1.952902
H	0.777890	2.704279	-2.211046
H	0.777890	2.704279	2.211046
C	-2.057577	-0.825085	-1.945700
C	-1.698309	0.594472	-2.000141
C	-0.831130	-1.651482	-1.952902
C	-2.057577	-0.825085	1.945700
C	-0.831130	-1.651482	1.952902
C	-1.698309	0.594472	2.000141
H	-0.777890	-2.704279	-2.211046
H	-0.777890	-2.704279	2.211046
C	-3.988708	0.446230	-1.863595
C	-2.894533	1.371389	-1.917753
C	-3.494853	-0.891318	-1.831102
C	-3.988708	0.446230	1.863595
C	-3.494853	-0.891318	1.831102
C	-2.894533	1.371389	1.917753
H	-2.975790	2.452686	-1.946198
H	-2.975790	2.452686	1.946198
H	-5.037571	0.725748	-1.823282
H	-5.037571	0.725748	1.823282
H	-4.101587	-1.789805	-1.790096
H	-4.101587	-1.789805	1.790096

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
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-58.223713	0.000000	0.000000
83.761794	2.473824	0.051939
112.470175	0.000000	0.000000
124.331594	200.804778	6.257972

1b-S

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V	2.437401	-0.028344	0.007478
V	-2.437401	0.028344	-0.007478
V	0.220332	1.027681	-0.028168
V	-0.220332	-1.027681	0.028168
C	4.205236	-0.390493	-1.359108
C	3.179695	-1.330669	-1.679548
C	3.718800	0.947801	-1.524668
C	2.061269	-0.556120	-2.115712
C	2.378172	0.848792	-2.021499
C	3.633544	-0.244417	1.850649
C	3.067654	1.075086	1.747724
C	2.606447	-1.233859	1.965336
C	1.636923	0.895803	1.877368
C	1.353591	-0.559250	2.015986
H	5.203537	-0.648579	-1.018112
H	3.267598	-2.410666	-1.658007
H	4.285095	1.852975	-1.335307
H	4.694607	-0.469855	1.794783
H	3.611912	2.011755	1.786440
H	2.763669	-2.306518	2.009344
C	0.074062	0.707293	-2.222653
C	1.149373	1.641697	-2.015948
C	0.622159	-0.666038	-2.165035
C	-0.622159	0.666038	2.165035
C	-0.074062	-0.707293	2.222653
C	0.397230	1.652520	2.019414
H	1.102541	2.720806	-2.139572
H	0.311789	2.718442	2.208226
C	-1.636923	-0.895803	-1.877368
C	-1.353591	0.559250	-2.015986
C	-0.397230	-1.652520	-2.019414
C	-2.378172	-0.848792	2.021499
C	-1.149373	-1.641697	2.015948
C	-2.061269	0.556120	2.115712
H	-0.311789	-2.718442	-2.208226
H	-1.102541	-2.720806	2.139572
C	-3.633544	0.244417	-1.850649
C	-2.606447	1.233859	-1.965336
C	-3.067654	-1.075086	-1.747724
C	-4.205236	0.390493	1.359108
C	-3.718800	-0.947801	1.524668
C	-3.179695	1.330669	1.679548
H	-2.763669	2.306518	-2.009344

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H	-3.267598	2.410666	1.658007
H	-4.694607	0.469855	-1.794783
H	-5.203537	0.648579	1.018112
H	-3.611912	-2.011755	-1.786440
H	-4.285095	-1.852975	1.335307

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
48.581145	70.788826	0.862006
64.584400	37.383900	0.605188
116.620736	0.000000	0.000000
133.782270	16.676272	0.559211
146.425566	0.000000	0.000000

1b-T

V	2.464004	0.142327	-0.046339
V	-2.487690	-0.173698	0.101624
V	-0.013107	0.952554	-0.106495
V	-0.178266	-1.155482	-0.004789
C	4.013374	0.111443	-1.673131
C	3.075052	-0.925614	-1.948661
C	3.347726	1.383234	-1.686221
C	1.813002	-0.294864	-2.164681
C	1.976430	1.146044	-2.018074
C	3.870606	0.030718	1.667671
C	3.194388	1.297187	1.682327
C	2.923391	-1.022121	1.844703
C	1.801901	1.038463	1.899759
C	1.638264	-0.418342	2.001818
H	5.071143	-0.038490	-1.481836
H	3.296612	-1.986992	-1.991024
H	3.822754	2.342590	-1.509939
H	4.940374	-0.105606	1.546285
H	3.671419	2.266487	1.582154
H	3.155198	-2.082198	1.863893
C	-0.289175	0.758348	-2.249766
C	0.677203	1.802054	-2.057177
C	0.388316	-0.551002	-2.236939

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C	-0.443570	0.645616	2.170837
C	0.221349	-0.675810	2.176137
C	0.503315	1.688280	1.991674
H	0.511919	2.871763	-2.151180
H	0.327086	2.753686	2.110027
C	-1.832018	-1.001643	-1.874649
C	-1.678834	0.480644	-1.940516
C	-0.536298	-1.635991	-2.088787
C	-2.052575	-1.047292	2.108441
C	-0.752835	-1.719169	2.074726
C	-1.871410	0.390090	2.174638
H	-0.361229	-2.677507	-2.345509
H	-0.585661	-2.778313	2.257288
C	-3.905053	-0.015560	-1.631160
C	-2.976227	1.058233	-1.763149
C	-3.228554	-1.278296	-1.669392
C	-4.075418	-0.019999	1.719991
C	-3.426178	-1.294727	1.795843
C	-3.125842	1.023144	1.920641
H	-3.221138	2.114915	-1.752769
H	-3.334755	2.087133	1.898707
H	-4.970921	0.108642	-1.462621
H	-5.131540	0.129423	1.516396
H	-3.701905	-2.253091	-1.624579
H	-3.911664	-2.257047	1.673682

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
43.732716	71.937102	0.788565
55.062743	15.579924	0.215031
66.340012	32.841811	0.546111
111.875205	92.591579	2.596471
123.340457	19.756012	0.610777

1c-S

V	2.824517	-0.058185	0.000000
V	-2.638001	0.171444	0.000000
V	0.707950	0.457057	0.000000

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V	-0.929133	-1.246379	0.000000
C	4.003340	-0.349661	-1.902026
C	2.920499	-1.281528	-1.889764
C	3.494950	0.986941	-1.832871
C	1.701048	-0.520348	-1.940655
C	2.052146	0.898946	-1.904949
C	4.003340	-0.349661	1.902026
C	3.494950	0.986941	1.832871
C	2.920499	-1.281528	1.889764
C	2.052146	0.898946	1.904949
C	1.701048	-0.520348	1.940655
H	5.056229	-0.616092	-1.917717
H	3.009785	-2.362281	-1.911470
H	4.090062	1.893780	-1.834507
H	5.056229	-0.616092	1.917717
H	4.090062	1.893780	1.834507
H	3.009785	-2.362281	1.911470
C	-0.236730	0.776330	-2.018052
C	0.828263	1.704622	-1.874393
C	0.247970	-0.603430	-1.963039
C	-0.236730	0.776330	2.018052
C	0.247970	-0.603430	1.963039
C	0.828263	1.704622	1.874393
H	0.767894	2.786160	-1.897219
H	0.767894	2.786160	1.897219
C	-2.068537	-0.701523	-2.003033
C	-1.687063	0.707581	-1.987850
C	-0.870721	-1.593479	-2.009162
C	-2.068537	-0.701523	2.003033
C	-0.870721	-1.593479	2.009162
C	-1.687063	0.707581	1.987850
H	-0.821129	-2.524159	-2.570540
H	-0.821129	-2.524159	2.570540
C	-3.965754	0.584659	-1.788778
C	-2.850712	1.498169	-1.819268
C	-3.500036	-0.756942	-1.882814
C	-3.965754	0.584659	1.788778
C	-3.500036	-0.756942	1.882814
C	-2.850712	1.498169	1.819268
H	-2.911533	2.579652	-1.770195
H	-2.911533	2.579652	1.770195
H	-5.006361	0.879587	-1.688887
H	-5.006361	0.879587	1.688887
H	-4.119169	-1.647233	-1.892679

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H	-4.119169	-1.647233	1.892679

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
76.883833	2.926978	0.056407
94.273332	15.221513	0.359687
113.234544	51.386106	1.458488
145.686155	10.393406	0.379537
154.684714	67.984983	2.635958

1c-T

V	2.816094	-0.159196	0.000000
V	-2.610840	0.204677	0.000000
V	0.662209	0.460715	0.000000
V	-0.893641	-1.291492	0.000000
C	3.998321	-0.322144	-1.913459
C	2.918800	-1.257268	-1.960932
C	3.489037	1.009201	-1.767189
C	1.699545	-0.494580	-1.955962
C	2.047500	0.926071	-1.847099
C	3.998321	-0.322144	1.913459
C	3.489037	1.009201	1.767189
C	2.918800	-1.257268	1.960932
C	2.047500	0.926071	1.847099
C	1.699545	-0.494580	1.955962
H	5.051866	-0.585696	-1.941612
H	3.010671	-2.333999	-2.054667
H	4.083718	1.914975	-1.721745
H	5.051866	-0.585696	1.941612
H	4.083718	1.914975	1.721745
H	3.010671	-2.333999	2.054667
C	-0.237993	0.799732	-2.019154
C	0.821079	1.734550	-1.815592
C	0.250246	-0.573579	-2.001667
C	-0.237993	0.799732	2.019154
C	0.250246	-0.573579	2.001667
C	0.821079	1.734550	1.815592
H	0.760364	2.815603	-1.855521

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H	0.760364	2.815603	1.855521
C	-2.059705	-0.699846	-1.996438
C	-1.690698	0.718074	-1.982513
C	-0.853609	-1.571311	-2.035205
C	-2.059705	-0.699846	1.996438
C	-0.853609	-1.571311	2.035205
C	-1.690698	0.718074	1.982513
H	-0.803728	-2.504523	-2.593044
H	-0.803728	-2.504523	2.593044
C	-3.972018	0.573215	-1.784081
C	-2.868681	1.494844	-1.834218
C	-3.489318	-0.762334	-1.869475
C	-3.972018	0.573215	1.784081
C	-3.489318	-0.762334	1.869475
C	-2.868681	1.494844	1.834218
H	-2.943426	2.575965	-1.786222
H	-2.943426	2.575965	1.786222
H	-5.015641	0.856431	-1.685217
H	-5.015641	0.856431	1.685217
H	-4.100202	-1.659104	-1.847358
H	-4.100202	-1.659104	1.847358

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
76.348144	1.049257	0.020080
129.078160	44.327327	1.434176
131.785188	90.976426	3.005201
138.935417	70.868454	2.467993
143.284711	74.506800	2.675924

2a-cis-S

V	3.059344	0.011022	0.000000
V	-3.111179	0.095241	0.000000
V	0.874282	0.730803	0.000000
V	-0.933714	-0.559142	0.000000
Cl	4.823080	-1.716329	0.000000
Cl	-3.433295	2.472954	0.000000

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C	3.878856	0.274214	-2.110573
C	2.981902	-0.852410	-2.079048
C	3.149481	1.473882	-1.945154
C	1.665392	-0.334304	-1.963041
C	1.745218	1.129466	-1.994034
C	3.878856	0.274214	2.110573
C	3.149481	1.473882	1.945154
C	2.981902	-0.852410	2.079048
C	1.745218	1.129466	1.994034
C	1.665392	-0.334304	1.963041
H	4.958028	0.197030	-2.182645
H	3.270326	-1.890682	-2.166615
H	3.565541	2.475790	-1.937713
H	4.958028	0.197030	2.182645
H	3.565541	2.475790	1.937713
H	3.270326	-1.890682	2.166615
C	-0.489266	0.560120	-1.972148
C	0.420718	1.699331	-1.912158
C	0.252276	-0.697215	-1.906059
C	-0.489266	0.560120	1.972148
C	0.252276	-0.697215	1.906059
C	0.420718	1.699331	1.912158
H	0.140389	2.741432	-2.010418
H	0.140389	2.741432	2.010418
C	-1.987129	-1.260187	-1.822188
C	-1.896988	0.193593	-1.986324
C	-0.656172	-1.824424	-1.707271
C	-1.987129	-1.260187	1.822188
C	-0.656172	-1.824424	1.707271
C	-1.896988	0.193593	1.986324
H	-0.391418	-2.874772	-1.701450
H	-0.391418	-2.874772	1.701450
C	-4.132151	-0.412796	-2.010933
C	-3.243515	0.685471	-2.153790
C	-3.392920	-1.578506	-1.674780
C	-4.132151	-0.412796	2.010933
C	-3.392920	-1.578506	1.674780
C	-3.243515	0.685471	2.153790
H	-3.523309	1.699124	-2.398292
H	-3.523309	1.699124	2.398292
H	-5.213362	-0.356054	-2.092975
H	-5.213362	-0.356054	2.092975
H	-3.812143	-2.564867	-1.506339
H	-3.812143	-2.564867	1.506339

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Intensities
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Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
19.212994	0.000000	0.000000
35.209908	1343.992505	11.861505
41.713599	165.376361	1.729136
86.245083	42.413531	0.916889
112.346801	28.502329	0.802637

2a-cis-T

V	3.234741	-0.197078	0.000000
V	-3.234741	0.197078	0.000000
V	0.930094	0.568668	0.000000
V	-0.930094	-0.568668	0.000000
Cl	4.965251	-1.846049	0.000000
Cl	-4.965251	1.846049	0.000000
C	4.005619	0.130876	-2.151610
C	3.059399	-0.948398	-2.105404
C	3.352782	1.357071	-1.912720
C	1.767482	-0.362083	-1.932156
C	1.926630	1.096848	-1.912914
C	4.005619	0.130876	2.151610
C	3.352782	1.357071	1.912720
C	3.059399	-0.948398	2.105404
C	1.926630	1.096848	1.912914
C	1.767482	-0.362083	1.932156
H	5.076457	0.004427	-2.268849
H	3.286027	-1.996176	-2.252305
H	3.828707	2.331780	-1.879093
H	5.076457	0.004427	2.268849
H	3.828707	2.331780	1.879093
H	3.286027	-1.996176	2.252305
C	-0.337142	0.650087	-1.882757
C	0.638333	1.738298	-1.790076
C	0.337142	-0.650087	-1.882757
C	-0.337142	0.650087	1.882757
C	0.337142	-0.650087	1.882757
C	0.638333	1.738298	1.790076

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H	0.422834	2.797885	-1.857659
H	0.422834	2.797885	1.857659
C	-1.926630	-1.096848	-1.912914
C	-1.767482	0.362083	-1.932156
C	-0.638333	-1.738298	-1.790076
C	-1.926630	-1.096848	1.912914
C	-0.638333	-1.738298	1.790076
C	-1.767482	0.362083	1.932156
H	-0.422834	-2.797885	-1.857659
H	-0.422834	-2.797885	1.857659
C	-4.005619	-0.130876	-2.151610
C	-3.059399	0.948398	-2.105404
C	-3.352782	-1.357071	-1.912720
C	-4.005619	-0.130876	2.151610
C	-3.352782	-1.357071	1.912720
C	-3.059399	0.948398	2.105404
H	-3.286027	1.996176	-2.252305
H	-3.286027	1.996176	2.252305
H	-5.076457	-0.004427	-2.268849
H	-5.076457	-0.004427	2.268849
H	-3.828707	-2.331780	-1.879093
H	-3.828707	-2.331780	1.879093

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
27.265517	274.191118	1.873895
44.180892	0.000000	0.000000
51.977570	162.720710	2.120005
54.603634	785.816163	10.755252
105.528169	49.240899	1.302484

2a-trans-S

V	0.539787	-1.049216	0.000000
V	-0.539787	1.049216	0.000000
V	-0.090993	-3.187607	0.000000
V	0.090993	3.187607	0.000000
Cl	-1.929847	4.527209	0.000000
Cl	1.929847	-4.527209	0.000000

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C	-0.817827	-3.938101	-2.070938
C	-1.610974	-2.808304	-1.702182
C	0.534411	-3.544682	-2.194863
C	-0.747762	-1.652946	-1.791412
C	0.624321	-2.113218	-2.001443
C	-0.817827	-3.938101	2.070938
C	0.534411	-3.544682	2.194863
C	-1.610974	-2.808304	1.702182
C	0.624321	-2.113218	2.001443
C	-0.747762	-1.652946	1.791412
H	-1.182392	-4.955168	-2.179337
H	-2.688487	-2.798794	-1.581854
H	1.358978	-4.201018	-2.431162
H	-1.182392	-4.955168	2.179337
H	1.358978	-4.201018	2.431162
H	-2.688487	-2.798794	1.581854
C	0.715549	0.193791	-1.827315
C	1.559160	-0.989924	-1.884255
C	-0.715549	-0.193791	-1.827315
C	0.715549	0.193791	1.827315
C	-0.715549	-0.193791	1.827315
C	1.559160	-0.989924	1.884255
H	2.626615	-1.017408	-2.068385
H	2.626615	-1.017408	2.068385
C	-0.624321	2.113218	-2.001443
C	0.747762	1.652946	-1.791412
C	-1.559160	0.989924	-1.884255
C	-0.624321	2.113218	2.001443
C	-1.559160	0.989924	1.884255
C	0.747762	1.652946	1.791412
H	-2.626615	1.017408	-2.068385
H	-2.626615	1.017408	2.068385
C	0.817827	3.938101	-2.070938
C	1.610974	2.808304	-1.702182
C	-0.534411	3.544682	-2.194863
C	0.817827	3.938101	2.070938
C	-0.534411	3.544682	2.194863
C	1.610974	2.808304	1.702182
H	2.688487	2.798794	-1.581854
H	2.688487	2.798794	1.581854
H	1.182392	4.955168	-2.179337
H	1.182392	4.955168	2.179337
H	-1.358978	4.201018	-2.431162
H	-1.358978	4.201018	2.431162

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Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
33.478626	0.000000	0.000000
35.346223	183.591412	1.626573
58.235555	93.199667	1.360444
66.598116	476.173126	7.948861
124.491086	1.414816	0.044149

2a-trans-T

V	0.624385	-1.069854	0.000000
V	-0.624385	1.069854	0.000000
V	-0.036623	-3.197311	0.000000
V	0.036623	3.197311	0.000000
Cl	-1.788553	4.786710	0.000000
Cl	1.788553	-4.786710	0.000000
C	-0.740756	-3.940639	-2.084898
C	-1.557600	-2.831736	-1.719018
C	0.607536	-3.523678	-2.210382
C	-0.712157	-1.662639	-1.789932
C	0.671001	-2.099185	-2.014374
C	-0.740756	-3.940639	2.084898
C	0.607536	-3.523678	2.210382
C	-1.557600	-2.831736	1.719018
C	0.671001	-2.099185	2.014374
C	-0.712157	-1.662639	1.789932
H	-1.081387	-4.968035	-2.174696
H	-2.635528	-2.843625	-1.603171
H	1.443978	-4.171336	-2.429436
H	-1.081387	-4.968035	2.174696
H	1.443978	-4.171336	2.429436
H	-2.635528	-2.843625	1.603171
C	0.707246	0.207296	-1.857488
C	1.572416	-0.951104	-1.926973
C	-0.707246	-0.207296	-1.857488
C	0.707246	0.207296	1.857488
C	-0.707246	-0.207296	1.857488
C	1.572416	-0.951104	1.926973

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H	2.643068	-0.949967	-2.094416
H	2.643068	-0.949967	2.094416
C	-0.671001	2.099185	-2.014374
C	0.712157	1.662639	-1.789932
C	-1.572416	0.951104	-1.926973
C	-0.671001	2.099185	2.014374
C	-1.572416	0.951104	1.926973
C	0.712157	1.662639	1.789932
H	-2.643068	0.949967	-2.094416
H	-2.643068	0.949967	2.094416
C	0.740756	3.940639	-2.084898
C	1.557600	2.831736	-1.719018
C	-0.607536	3.523678	-2.210382
C	0.740756	3.940639	2.084898
C	-0.607536	3.523678	2.210382
C	1.557600	2.831736	1.719018
H	2.635528	2.843625	-1.603171
H	2.635528	2.843625	1.603171
H	1.081387	4.968035	-2.174696
H	1.081387	4.968035	2.174696
H	-1.443978	4.171336	-2.429436
H	-1.443978	4.171336	2.429436

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
27.805820	536.107833	3.736508
32.163612	0.000000	0.000000
51.660252	83.595625	1.082476
70.706082	449.311134	7.963097
98.821833	0.000000	0.000000

2b-S

V	2.457403	-0.023302	-0.047453
V	-2.457403	0.023302	0.047453
V	0.310876	1.087807	0.204506
V	-0.310876	-1.087807	-0.204506
Cl	1.520855	-2.674167	-0.017890
Cl	-1.520855	2.674167	0.017890

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C	4.003212	0.122418	-1.693833
C	3.115737	-0.933648	-2.020834
C	3.275498	1.354672	-1.601788
C	1.810005	-0.358475	-2.173589
C	1.912815	1.076549	-1.951101
C	3.926116	0.178539	1.649504
C	3.212236	1.414213	1.596723
C	3.025819	-0.892292	1.948878
C	1.847404	1.136385	1.957366
C	1.729285	-0.316685	2.089123
H	5.068101	0.008027	-1.516810
H	3.380168	-1.980162	-2.106975
H	3.704296	2.325073	-1.376286
H	4.992793	0.065701	1.483055
H	3.648756	2.391730	1.423151
H	3.282034	-1.941428	2.021260
C	-0.311576	0.606426	-2.159350
C	0.601098	1.689623	-1.951938
C	0.392681	-0.672533	-2.288163
C	-0.392681	0.672533	2.288163
C	0.311576	-0.606426	2.159350
C	0.553500	1.761333	2.179821
H	0.373682	2.744505	-2.050530
H	0.370933	2.817541	2.338454
C	-1.847404	-1.136385	-1.957366
C	-1.729285	0.316685	-2.089123
C	-0.553500	-1.761333	-2.179821
C	-1.912815	-1.076549	1.951101
C	-0.601098	-1.689623	1.951938
C	-1.810005	0.358475	2.173589
H	-0.370933	-2.817541	-2.338454
H	-0.373682	-2.744505	2.050530
C	-3.926116	-0.178539	-1.649504
C	-3.025819	0.892292	-1.948878
C	-3.212236	-1.414213	-1.596723
C	-4.003212	-0.122418	1.693833
C	-3.275498	-1.354672	1.601788
C	-3.115737	0.933648	2.020834
H	-3.282034	1.941428	-2.021260
H	-3.380168	1.980162	2.106975
H	-4.992793	-0.065701	-1.483055
H	-5.068101	-0.008027	1.516810
H	-3.648756	-2.391730	-1.423151
H	-3.704296	-2.325073	1.376286

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Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
-15.253111	0.000000	0.000000
69.078107	0.000000	0.000000
92.952194	79.759681	1.858323
127.111819	123.824676	3.945220
130.890949	0.000000	0.000000

2b-T

V	2.476989	0.265955	-0.109703
V	-2.476989	-0.265955	0.109703
V	0.164883	1.126336	0.225900
V	-0.164883	-1.126336	-0.225900
Cl	1.184081	-3.061802	0.003274
Cl	-1.184081	3.061802	-0.003274
C	4.056048	0.151284	-1.738881
C	3.154745	-0.926849	-1.960008
C	3.354754	1.398344	-1.799454
C	1.868949	-0.357968	-2.212640
C	1.989802	1.092944	-2.094559
C	3.867422	0.214846	1.681030
C	3.171358	1.454211	1.715559
C	2.950271	-0.876978	1.763983
C	1.776166	1.153078	1.940068
C	1.649792	-0.313091	1.926947
H	5.116108	0.040953	-1.530458
H	3.398497	-1.982098	-1.915255
H	3.791953	2.381896	-1.663018
H	4.940578	0.111192	1.547658
H	3.622159	2.439891	1.673297
H	3.189471	-1.932248	1.710627
C	-0.244828	0.618418	-2.093872
C	0.676640	1.692182	-1.983223
C	0.453351	-0.671025	-2.296490
C	-0.453351	0.671025	2.296490
C	0.244828	-0.618418	2.093872
C	0.484179	1.752538	2.248122

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H	0.435693	2.746498	-2.033223
H	0.294954	2.801044	2.439814
C	-1.776166	-1.153078	-1.940068
C	-1.649792	0.313091	-1.926947
C	-0.484179	-1.752538	-2.248122
C	-1.989802	-1.092944	2.094559
C	-0.676640	-1.692182	1.983223
C	-1.868949	0.357968	2.212640
H	-0.294954	-2.801044	-2.439814
H	-0.435693	-2.746498	2.033223
C	-3.867422	-0.214846	-1.681030
C	-2.950271	0.876978	-1.763983
C	-3.171358	-1.454211	-1.715559
C	-4.056048	-0.151284	1.738881
C	-3.354754	-1.398344	1.799454
C	-3.154745	0.926849	1.960008
H	-3.189471	1.932248	-1.710627
H	-3.398497	1.982098	1.915255
H	-4.940578	-0.111192	-1.547658
H	-5.116108	-0.040953	1.530458
H	-3.622159	-2.439891	-1.673297
H	-3.791953	-2.381896	1.663018

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
72.390058	34.415782	0.624474
88.083107	0.000000	0.000000
95.709835	302.524924	7.257646
116.112254	0.000000	0.000000
120.093129	49.718352	1.496625

3a-cis-S

V	0.599359	-0.881997	0.000000
V	-0.599359	0.881997	0.000000
V	0.010913	-3.166092	0.000000
V	-0.010913	3.166092	0.000000
C	-1.616341	-4.172067	0.000000
C	1.616341	4.172067	0.000000

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O	-2.619856	-4.778277	0.000000
O	2.619856	4.778277	0.000000
C	0.273586	-4.028183	-2.069186
C	-0.832955	-3.104708	-2.078636
C	1.478239	-3.323188	-1.797796
C	-0.295168	-1.784001	-1.917584
C	1.165241	-1.898638	-1.883074
C	0.273586	-4.028183	2.069186
C	1.478239	-3.323188	1.797796
C	-0.832955	-3.104708	2.078636
C	1.165241	-1.898638	1.883074
C	-0.295168	-1.784001	1.917584
H	0.189419	-5.100308	-2.213819
H	-1.860290	-3.341518	-2.326051
H	2.471090	-3.758754	-1.774938
H	0.189419	-5.100308	2.213819
H	2.471090	-3.758754	1.774938
H	-1.860290	-3.341518	2.326051
C	0.638208	0.361151	-1.895329
C	1.759078	-0.578888	-1.782934
C	-0.638208	-0.361151	-1.895329
C	0.638208	0.361151	1.895329
C	-0.638208	-0.361151	1.895329
C	1.759078	-0.578888	1.782934
H	2.811112	-0.329715	-1.850464
H	2.811112	-0.329715	1.850464
C	-1.165241	1.898638	-1.883074
C	0.295168	1.784001	-1.917584
C	-1.759078	0.578888	-1.782934
C	-1.165241	1.898638	1.883074
C	-1.759078	0.578888	1.782934
C	0.295168	1.784001	1.917584
H	-2.811112	0.329715	-1.850464
H	-2.811112	0.329715	1.850464
C	-0.273586	4.028183	-2.069186
C	0.832955	3.104708	-2.078636
C	-1.478239	3.323188	-1.797796
C	-0.273586	4.028183	2.069186
C	-1.478239	3.323188	1.797796
C	0.832955	3.104708	2.078636
H	1.860290	3.341518	-2.326051
H	1.860290	3.341518	2.326051
H	-0.189419	5.100308	-2.213819
H	-0.189419	5.100308	2.213819

H	-2.471090	3.758754	-1.774938
H	-2.471090	3.758754	1.774938

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
48.141842	321.928562	3.884725
50.154828	0.000000	0.000000
63.249497	0.141565	0.002244
85.131541	100.652875	2.147804
111.749740	0.049159	0.001377

3a-cis-T

V	0.609051	-0.865503	0.000000
V	-0.609051	0.865503	0.000000
V	-0.074920	-3.275740	0.000000
V	0.074920	3.275740	0.000000
C	-1.543609	-4.506096	0.000000
C	1.543609	4.506096	0.000000
O	-2.440477	-5.256278	0.000000
O	2.440477	5.256278	0.000000
C	0.180499	-4.020696	-2.108244
C	-0.909855	-3.076803	-2.091851
C	1.401207	-3.342853	-1.840953
C	-0.335831	-1.775956	-1.918697
C	1.122970	-1.914875	-1.898608
C	0.180499	-4.020696	2.108244
C	1.401207	-3.342853	1.840953
C	-0.909855	-3.076803	2.091851
C	1.122970	-1.914875	1.898608
C	-0.335831	-1.775956	1.918697
H	0.081562	-5.084764	-2.297292
H	-1.945625	-3.294795	-2.322685
H	2.383576	-3.803211	-1.828535
H	0.081562	-5.084764	2.297292
H	2.383576	-3.803211	1.828535
H	-1.945625	-3.294795	2.322685
C	0.646688	0.350667	-1.893892
C	1.746069	-0.616039	-1.813013

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C	-0.646688	-0.350667	-1.893892
C	0.646688	0.350667	1.893892
C	-0.646688	-0.350667	1.893892
C	1.746069	-0.616039	1.813013
H	2.803630	-0.391106	-1.881534
H	2.803630	-0.391106	1.881534
C	-1.122970	1.914875	-1.898608
C	0.335831	1.775956	-1.918697
C	-1.746069	0.616039	-1.813013
C	-1.122970	1.914875	1.898608
C	-1.746069	0.616039	1.813013
C	0.335831	1.775956	1.918697
H	-2.803630	0.391106	-1.881534
H	-2.803630	0.391106	1.881534
C	-0.180499	4.020696	-2.108244
C	0.909855	3.076803	-2.091851
C	-1.401207	3.342853	-1.840953
C	-0.180499	4.020696	2.108244
C	-1.401207	3.342853	1.840953
C	0.909855	3.076803	2.091851
H	1.945625	3.294795	-2.322685
H	1.945625	3.294795	2.322685
H	-0.081562	5.084764	-2.297292
H	-0.081562	5.084764	2.297292
H	-2.383576	3.803211	-1.828535
H	-2.383576	3.803211	1.828535

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
29.944129	316.308479	2.374109
52.565812	153.996601	2.029049
56.948304	233.046335	3.326604
56.990807	0.000000	0.000000
71.611755	8.890615	0.159586

3a-trans-S

V	0.442370	-1.028245	0.000000
V	-0.442370	1.028245	0.000000

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V	-0.256875	-3.252868	0.000000
V	0.256875	3.252868	0.000000
C	0.711401	-4.924856	0.000000
C	-0.711401	4.924856	0.000000
O	1.310498	-5.928916	0.000000
O	-1.310498	5.928916	0.000000
C	-0.887714	-3.932779	-2.060306
C	-1.671933	-2.788019	-1.761615
C	0.507275	-3.565168	-2.092192
C	-0.773448	-1.643368	-1.806777
C	0.600003	-2.131180	-1.955214
C	-0.887714	-3.932779	2.060306
C	0.507275	-3.565168	2.092192
C	-1.671933	-2.788019	1.761615
C	0.600003	-2.131180	1.955214
C	-0.773448	-1.643368	1.806777
H	-1.270587	-4.936950	-2.208168
H	-2.754207	-2.752330	-1.713826
H	1.328009	-4.226917	-2.342652
H	-1.270587	-4.936950	2.208168
H	1.328009	-4.226917	2.342652
H	-2.754207	-2.752330	1.713826
C	0.715900	0.185214	-1.852259
C	1.537342	-1.018570	-1.843172
C	-0.715900	-0.185214	-1.852259
C	0.715900	0.185214	1.852259
C	-0.715900	-0.185214	1.852259
C	1.537342	-1.018570	1.843172
H	2.612621	-1.060812	-1.968100
H	2.612621	-1.060812	1.968100
C	-0.600003	2.131180	-1.955214
C	0.773448	1.643368	-1.806777
C	-1.537342	1.018570	-1.843172
C	-0.600003	2.131180	1.955214
C	-1.537342	1.018570	1.843172
C	0.773448	1.643368	1.806777
H	-2.612621	1.060812	-1.968100
H	-2.612621	1.060812	1.968100
C	0.887714	3.932779	-2.060306
C	1.671933	2.788019	-1.761615
C	-0.507275	3.565168	-2.092192
C	0.887714	3.932779	2.060306
C	-0.507275	3.565168	2.092192
C	1.671933	2.788019	1.761615

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H	2.754207	2.752330	-1.713826
H	2.754207	2.752330	1.713826
H	1.270587	4.936950	-2.208168
H	1.270587	4.936950	2.208168
H	-1.328009	4.226917	-2.342652
H	-1.328009	4.226917	2.342652

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
45.135067	161.180659	1.823497
52.925142	0.000000	0.000000
68.370205	100.136751	1.716084
73.135614	0.741903	0.013600
95.067239	1.409421	0.033585

3a-trans-T

V	0.486708	-1.042004	0.000000
V	-0.486708	1.042004	0.000000
V	-0.246789	-3.260338	0.000000
V	0.246789	3.260338	0.000000
C	0.686976	-4.954521	0.000000
C	-0.686976	4.954521	0.000000
O	1.276026	-5.964206	0.000000
O	-1.276026	5.964206	0.000000
C	-0.881376	-3.938490	-2.052609
C	-1.666098	-2.793924	-1.748903
C	0.513218	-3.564949	-2.105829
C	-0.772471	-1.647589	-1.801743
C	0.600089	-2.133551	-1.974572
C	-0.881376	-3.938490	2.052609
C	0.513218	-3.564949	2.105829
C	-1.666098	-2.793924	1.748903
C	0.600089	-2.133551	1.974572
C	-0.772471	-1.647589	1.801743
H	-1.263660	-4.943299	-2.197102
H	-2.747965	-2.762005	-1.689801
H	1.333942	-4.225284	-2.360264
H	-1.263660	-4.943299	2.197102

H	1.333942	-4.225284	2.360264
H	-2.747965	-2.762005	1.689801
C	0.717684	0.186773	-1.834993
C	1.533366	-1.021284	-1.875968
C	-0.717684	-0.186773	-1.834993
C	0.717684	0.186773	1.834993
C	-0.717684	-0.186773	1.834993
C	1.533366	-1.021284	1.875968
H	2.608858	-1.068076	-2.002811
H	2.608858	-1.068076	2.002811
C	-0.600089	2.133551	-1.974572
C	0.772471	1.647589	-1.801743
C	-1.533366	1.021284	-1.875968
C	-0.600089	2.133551	1.974572
C	-1.533366	1.021284	1.875968
C	0.772471	1.647589	1.801743
H	-2.608858	1.068076	-2.002811
H	-2.608858	1.068076	2.002811
C	0.881376	3.938490	-2.052609
C	1.666098	2.793924	-1.748903
C	-0.513218	3.564949	-2.105829
C	0.881376	3.938490	2.052609
C	-0.513218	3.564949	2.105829
C	1.666098	2.793924	1.748903
H	2.747965	2.762005	-1.689801
H	2.747965	2.762005	1.689801
H	1.263660	4.943299	-2.197102
H	1.263660	4.943299	2.197102
H	-1.333942	4.225284	-2.360264
H	-1.333942	4.225284	2.360264

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
48.414137	205.473659	2.493483
58.186183	0.000000	0.000000
70.499097	5.928303	0.104759
84.171548	66.698512	1.407212
91.622022	2.198650	0.050493

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3b-S

V	2.450294	0.009289	-0.063782
V	-2.450294	-0.009289	0.063782
V	0.250662	1.069974	0.208000
V	-0.250662	-1.069974	-0.208000
C	1.659578	-2.099326	0.017312
C	-1.659578	2.099326	-0.017312
O	2.077739	-3.208531	-0.041642
O	-2.077739	3.208531	0.041642
C	3.993687	0.140925	-1.667056
C	3.110180	-0.921935	-2.006513
C	3.266596	1.377499	-1.602972
C	1.816859	-0.337680	-2.196719
C	1.904066	1.099962	-1.953346
C	3.912549	0.196724	1.656664
C	3.207124	1.432887	1.616512
C	3.006559	-0.883094	1.912468
C	1.831591	1.160204	1.940617
C	1.716676	-0.285559	2.081141
H	5.057144	0.029736	-1.479642
H	3.384165	-1.963617	-2.123416
H	3.694693	2.347906	-1.374807
H	4.980238	0.085799	1.493471
H	3.651865	2.407785	1.447111
H	3.273769	-1.922892	2.053792
C	-0.310709	0.592998	-2.163287
C	0.575825	1.698013	-1.933961
C	0.404400	-0.671978	-2.307353
C	-0.404400	0.671978	2.307353
C	0.310709	-0.592998	2.163287
C	0.513689	1.781796	2.166780
H	0.334090	2.744232	-2.095420
H	0.332018	2.833092	2.363024
C	-1.831591	-1.160204	-1.940617
C	-1.716676	0.285559	-2.081141
C	-0.513689	-1.781796	-2.166780
C	-1.904066	-1.099962	1.953346
C	-0.575825	-1.698013	1.933961
C	-1.816859	0.337680	2.196719
H	-0.332018	-2.833092	-2.363024
H	-0.334090	-2.744232	2.095420
C	-3.912549	-0.196724	-1.656664
C	-3.006559	0.883094	-1.912468

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C	-3.207124	-1.432887	-1.616512
C	-3.993687	-0.140925	1.667056
C	-3.266596	-1.377499	1.602972
C	-3.110180	0.921935	2.006513
H	-3.273769	1.922892	-2.053792
H	-3.384165	1.963617	2.123416
H	-4.980238	-0.085799	-1.493471
H	-5.057144	-0.029736	1.479642
H	-3.651865	-2.407785	-1.447111
H	-3.694693	-2.347906	1.374807

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
68.286345	615.833528	10.540841
69.449959	72.223989	1.257279
102.926412	0.000000	0.000000
119.076911	0.000000	0.000000
123.842088	107.060177	3.323336

3b-T

V	2.503389	-0.148326	-0.000925
V	-2.560891	0.127629	0.000365
V	-0.046812	1.521941	0.015646
V	-0.084183	-0.751393	-0.008045
C	2.121211	-2.056251	-0.020856
C	-2.152258	2.014567	0.019781
O	2.130598	-3.232106	-0.033066
O	-1.834781	3.175527	0.031157
C	3.985925	0.131814	-1.655170
C	3.106742	-0.945795	-1.981856
C	3.239374	1.351070	-1.603403
C	1.785762	-0.381788	-2.104414
C	1.884434	1.059372	-1.928521
C	3.985133	0.097605	1.659592
C	3.238558	1.317627	1.632788
C	3.105822	-0.986613	1.963314
C	1.883428	1.019201	1.950996
C	1.784740	-0.425295	2.096857

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H	5.057569	0.042129	-1.511156
H	3.408519	-1.967640	-2.178988
H	3.657240	2.329742	-1.387413
H	5.056882	0.011081	1.514341
H	3.656626	2.300557	1.437524
H	3.407519	-2.012340	2.139308
C	-0.330141	0.554883	-2.178330
C	0.568633	1.703861	-2.015510
C	0.370750	-0.716270	-2.186290
C	-0.331303	0.509552	2.188884
C	0.369719	-0.761423	2.170805
C	0.567513	1.661697	2.050562
H	0.409912	2.669526	-2.498626
H	0.408482	2.616983	2.553792
C	-1.855030	-1.163196	-1.820870
C	-1.745811	0.256266	-2.120645
C	-0.542177	-1.800928	-1.888410
C	-1.855775	-1.200782	1.794698
C	-0.542910	-1.839677	1.849889
C	-1.746939	0.212119	2.124077
H	-0.354621	-2.865097	-1.979495
H	-0.355248	-2.905489	1.918748
C	-3.965111	-0.186034	-1.710391
C	-3.049102	0.844669	-2.076208
C	-3.240164	-1.410223	-1.526113
C	-3.965956	-0.221891	1.703396
C	-3.240683	-1.441839	1.493912
C	-3.050322	0.801086	2.091210
H	-3.316070	1.867993	-2.314465
H	-3.317625	1.819160	2.350638
H	-5.040785	-0.069692	-1.630564
H	-5.041607	-0.104111	1.625485
H	-3.688104	-2.367866	-1.285098
H	-3.688293	-2.394302	1.232593

Intensities
==========

Frequency cm^{-1}	Dipole Strength 1e-40 esu^2 cm^2	Absorption Intensity km/mole
74.697405	25.402584	0.475622
97.270456	94.363930	2.300727
112.051312	3.396138	0.095385

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121.771879	1.875014	0.057231
129.228012	1.649845	0.053441