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SUPPLEMENTARY DATA

to:

Valley ridge inflection points on the potential energy surfaces of H_2S, H_2Se, and H_2CO

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in: PCCP Ref: B102053F

Table 1 VRI points of the PES of H_2S

$\alpha/^o$	r_1=r_2/Å	Energy/h
[a]24.68821	1.76406	-398.68879605
25.11762	1.72758	-398.69210212
25.74953	1.66752	-398.69722640
25.81942	1.66013	-398.69779997
26.04784	1.63440	-398.69964764
26.50428	1.57090	-398.70278357
26.85439	1.49166	-398.70215498
39.91628	1.96968	-398.63920097
40.32877	1.91169	-398.65342568
42.10016	1.83388	-398.67315673
45.91104	1.77936	-398.68932038
47.41455	1.76963	-398.69306128
50.07875	1.75943	-398.69810798
52.87467	1.75445	-398.70206621
55.34116	1.75289	-398.70483251
58.26607	1.75315	-398.70748879
60.20786	1.75416	-398.70895688
65.05229	1.75819	-398.71181300
69.92677	1.76314	-398.71377584
74.88350	1.76792	-398.71505841
79.84608	1.77188	-398.71576512
84.88220	1.77461	-398.71597366
89.95977	1.77607	-398.71570753
98.01821	1.77559	-398.71433518
104.92554	1.77248	-398.71221735
108.25255	1.77013	-398.71087373
110.26206	1.76845	-398.70995636
112.10615	1.76673	-398.70904262
115.24604	1.76345	-398.70732382
117.41499	1.76091	-398.70601303
119.73508	1.75797	-398.70449566
125.01116	1.75043	-398.70058002
129.77923	1.74266	-398.69645230
134.46747	1.73425	-398.69180475
140.83810	1.72184	-398.68446973
145.50974	1.71232	-398.67827436
150.53033	1.70211	-398.67077013
155.55900	1.69252	-398.66229242
160.61110	1.68453	-398.65270225
165.80332	1.67976	-398.64155219
168.43851	1.67957	-398.63528175

[a]VRI point near the valley path to dissociation H_2+S.

Table 2 VRI points of the PES of H_2Se

$\alpha/^o$	r_1=r_2/Å	Energy/h
19.92072	2.16079	-2389.58691443
[a]22.68337	1.88371	-2389.59038591
23.40302	1.81231	-2389.59032579
24.11892	1.73545	-2389.58892416
24.70084	1.66124	-2389.58520926
25.09317	1.59475	-2389.57862393
25.34239	1.53006	-2389.56775658
41.17113	2.33216	-2389.50127513
41.68914	2.18040	-2389.53150558
42.49826	2.12237	-2389.54324469
43.29082	2.09035	-2389.54995356
45.32173	2.04814	-2389.55970721
45.81843	2.04240	-2389.56125616
47.08381	2.03244	-2389.56435648
49.73176	2.02501	-2389.56835813
52.11878	2.02637	-2389.57034968
54.94399	2.03206	-2389.57170543
59.64516	2.04377	-2389.57289860
65.30049	2.05616	-2389.57370214
70.18801	2.06452	-2389.57413984
75.37310	2.07123	-2389.57438655
80.20568	2.07566	-2389.57441845
84.62357	2.07822	-2389.57428199
90.00261	2.07944	-2389.57390076
94.92125	2.07873	-2389.57334352
99.82388	2.07625	-2389.57258362
104.68973	2.07202	-2389.57161863
109.85781	2.06556	-2389.57034937
114.94575	2.05716	-2389.56883272
119.92876	2.04694	-2389.56706192
125.11594	2.03416	-2389.56487724
129.70887	2.02098	-2389.56260621
134.78872	2.00436	-2389.55966070
139.45544	1.98722	-2389.55647750
147.74239	1.95260	-2389.54940823
151.91734	1.93338	-2389.54499224
155.89140	1.91425	-2389.54013824
159.69634	1.89550	-2389.53480818
164.97224	1.86961	-2389.52615299
169.81270	1.84732	-2389.51675209
173.86036	1.83096	-2389.50769149
176.04597	1.82309	-2389.50229344

[a]VRI point near the valley path to dissociation H_2+Se.

Table 3 VRI points of the PES of H_2CO[a]

α_1=α_2/^{o}	r_1=r_2/Å	Energy /h
85.35780	0.98479	-114.04881039
78.27256	1.04806	-114.03212458
77.96691	1.05909	-114.03143207
[b]77.58233	1.10066	-114.02895538
77.88002	1.14674	-114.02453010
77.94265	1.15240	-114.02381301
78.51633	1.19605	-114.01697475
79.16498	1.24024	-114.00788842
79.77662	1.28245	-113.99753753
80.22901	1.31559	-113.98852126
81.01760	1.38057	-113.96926563
81.78338	1.45917	-113.94453131
84.52847	1.48221	-113.94772335
86.82421	1.48172	-113.95699125
90.03152	1.48225	-113.96889543
95.03390	1.48542	-113.98505294
100.02354	1.49047	-113.99829276
105.00601	1.49623	-114.00872390
110.00744	1.50132	-114.01655029
115.01070	1.50411	-114.02198449
[c]120.01317	1.50279	-114.02536205
124.96546	1.49526	-114.02704337
129.88821	1.47890	-114.02740404
134.80962	1.45028	-114.02652620
[d]139.78114	1.40613	-114.02341797
144.91786	1.34593	-114.01447471
149.54075	1.28282	-113.99714283
152.25024	1.23956	-113.98145865
153.73578	1.17859	-113.97382455
152.78126	1.14131	-113.98546294
151.88745	1.12281	-113.99449165
150.52429	1.10199	-114.00693220
147.62534	1.07121	-114.02991647

α_1=α_2/^{o}	r_1=r_2/Å	Energy /h
158.96699	1.39292	-113.87614879
158.68203	1.32513	-113.89468518
158.43686	1.26278	-113.90881996
158.52611	1.23289	-113.91154936
158.93187	1.20886	-113.90825243
161.19394	1.14989	-113.87300658
82.36236	1.54818	-113.91620036
82.08089	1.50254	-113.93057614
81.34220	1.48508	-113.93354922
80.67366	1.48559	-113.93053386
79.24035	1.48742	-113.92373214
77.36695	1.49072	-113.91437636
74.38261	1.49835	-113.89838776
73.38893	1.50168	-113.89274774
71.20685	1.51073	-113.87975071
68.36373	1.52732	-113.86135052
72.27228	1.53806	-113.87507348
71.54667	1.50347	-113.88382880
70.36394	1.45116	-113.89734026
69.13926	1.39715	-113.91169554
67.92549	1.30541	-113.93883822
68.72689	1.25465	-113.95837708
72.60492	1.19440	-113.99173833
76.78111	1.16016	-114.01740663
77.94265	1.15240	-114.02381301
84.00758	1.11799	-114.05372164
[e]87.90503	1.09903	-114.07035925
101.55797	1.03713	-114.11373274

[a]r_3 is fixed to the value of 1.460Å.

[b]VRI point projection of the valley path of symmetric bending, at r_3≈1.50Å. The zero eigenvector is an anti-symmetric bend.

[c]VRI point near the valley path to the dissociation of H + CO + H, at r_3=1.189 5Å. The zero eigenvector is an anti-symmetric stretch.

[d]VRI point projection of the valley path to the dissociation of H_2 + CO, at r_3≈q1.646 5Å. The zero eigenvector is an anti-symmetric stretch.

[e]VRI point projection of the valley path of symmetric bending, at r_3≈1.632Å. The zero eigenvector is the book mode.